



# Geant4 for Microdosimetry

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*on behalf of the Geant4-DNA Team*

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RADAM06

Groningen, 6-9 June 2006

# Geant 4

**Object Oriented Toolkit**  
for the simulation of particle interactions with matter

also...

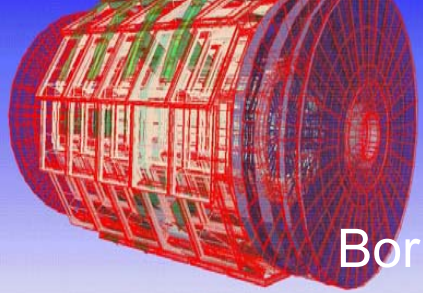
An experiment of  
**distributed software production and management**

An experiment of application of  
**rigorous software engineering methodologies**  
and **object oriented technology**  
to the particle physics environment

R&D phase: **RD44**, 1994 - 1998  
1<sup>st</sup> release: December 1998  
2 new releases/year since then

<http://cern.ch/geant4>  
<http://www.ge.infn.it/geant4>

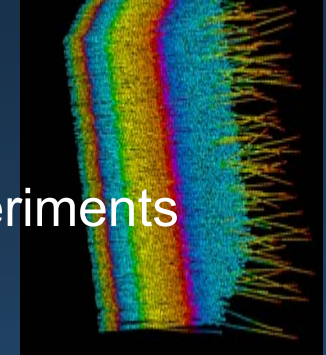
Courtesy CMS Collaboration



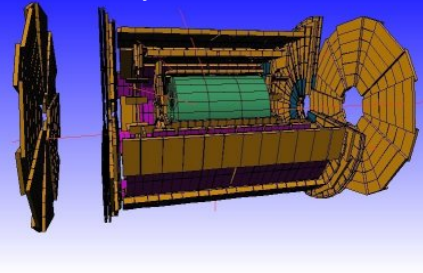
# Geant 4

Born from the requirements of large scale HEP experiments

Courtesy K. Amako et al., KEK



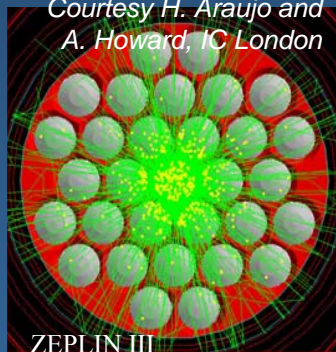
Courtesy ATLAS Collaboration



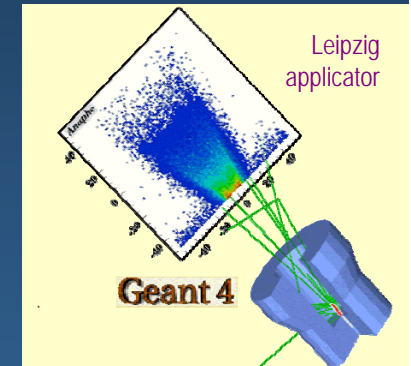
Widely used also in

- Space science and astrophysics
- Medical physics, nuclear medicine
- Radiation protection
- Accelerator physics
- Pest control, food irradiation
- Humanitarian projects, security
- etc.
- Technology transfer to industry, hospitals

Courtesy H. Araujo and A. Howard, IC London

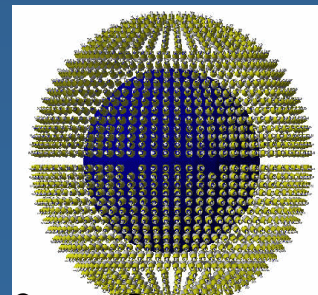


ZEPLIN III



Leipzig applicator

Geant 4



Courtesy Borexino



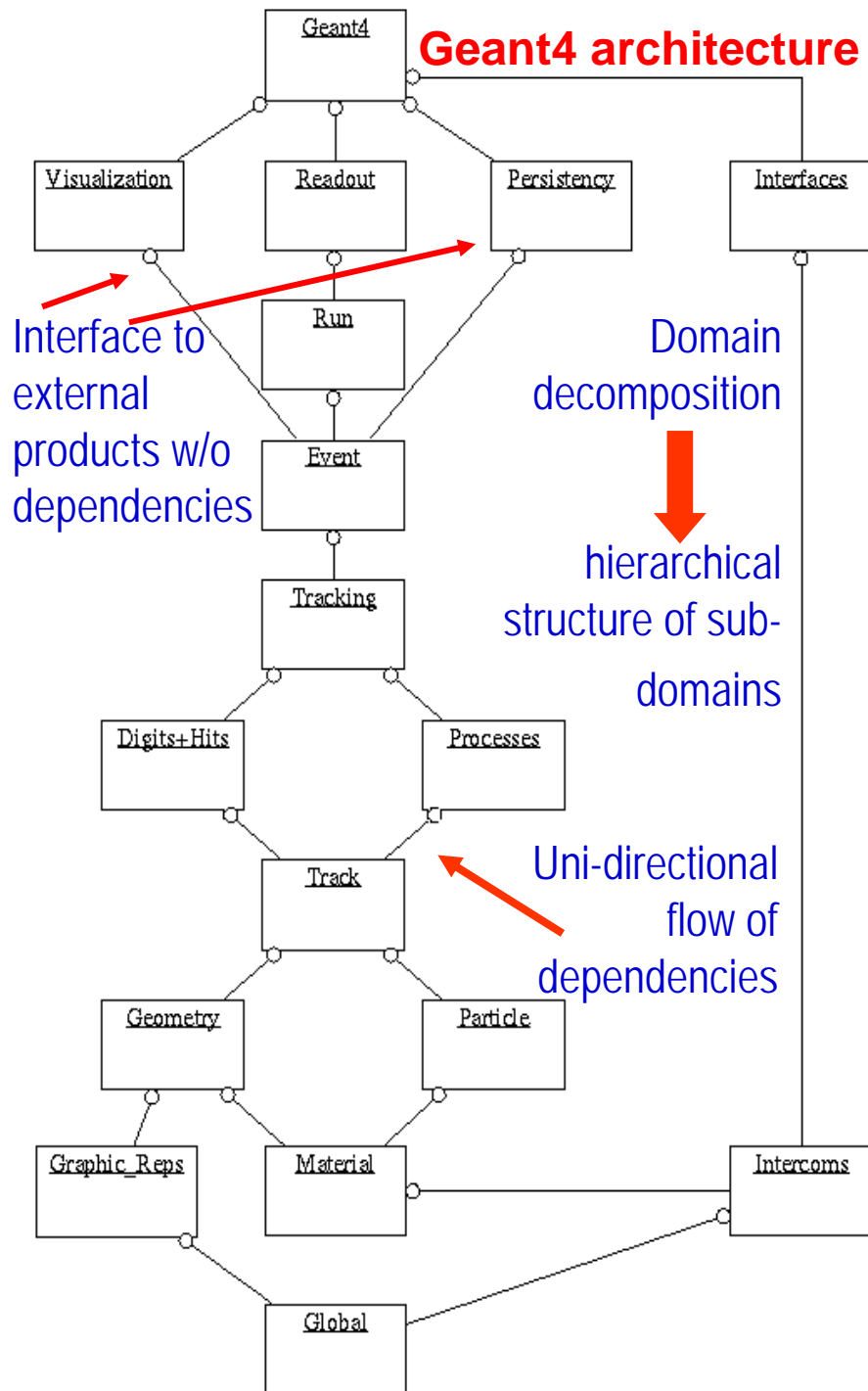
Courtesy R. Nartallo et al., ESA

INFN Genova

**Most cited  
“engineering”  
publication  
in the past 2 years!**

Courtesy GATE Collaboration





# Geant 4 in a nutshell

## ● Rigorous software engineering

- Iterative-incremental software process
- Object oriented methods
- Quality assurance

## ● Geometry

- Powerful and versatile geometry modelling
- Multiple solid representations handled through the same abstract interface  
(*CSG, STEP compliant solids, BREPs*)
- Simple placements, parameterised volumes, replicas, assembly-volumes etc.
- Boolean operations on solids

## ● Physics independent from tracking

## ● Subject to rigorous, quantitative validation

## ● Electromagnetic physics

- Standard, Low-Energy, Muon, Optical etc.

## ● Hadronic physics

- Parameterised, data-/theory-driven models

## ● Interactive capabilities

- Visualisation, UI/GUI
- Multiple drivers to external systems



~100 members



# Geant4 Collaboration



MoU based

Development, Distribution and User Support of Geant4

Major physics laboratories:

CERN, KEK, SLAC, TRIUMF, TJNL

European Space Agency:

ESA

National Institutes:

INFN, IN2P3, PPARC

Universities:

Budker Inst., Frankfurt, Karolinska Inst., Helsinki, Lebedev Inst., LIP, Lund, Northeastern *etc.*

Maria Grazia Pia, INFN Genova



# Multi-disciplinary application environment

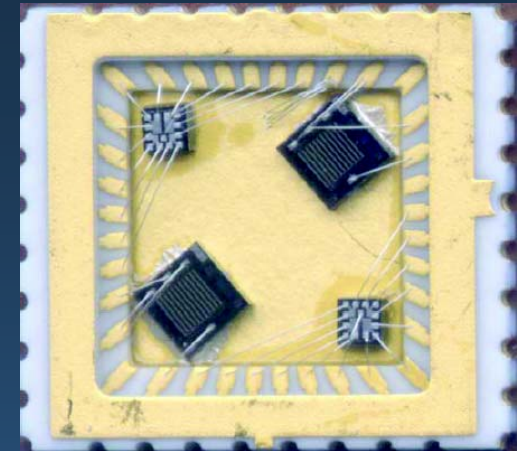
## Dosimetry



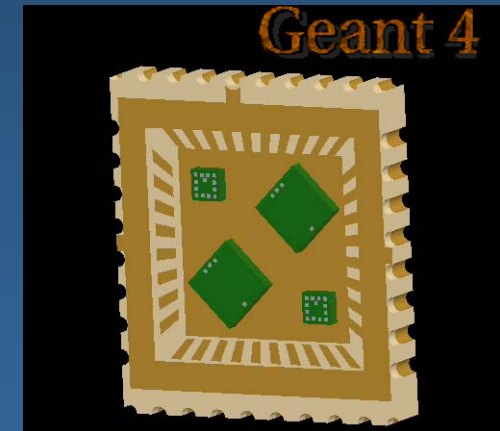
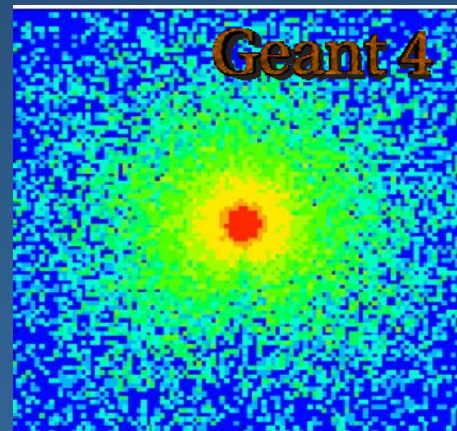
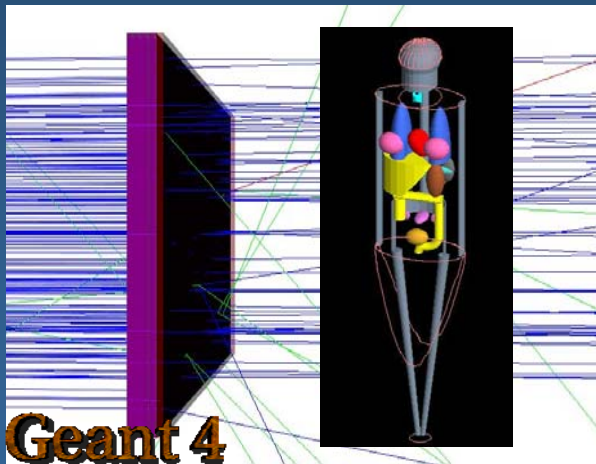
Space science



Radiotherapy



Effects on components



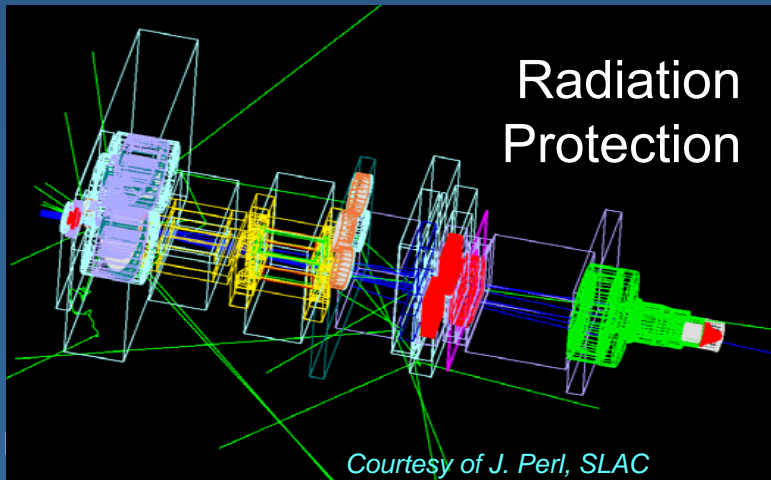
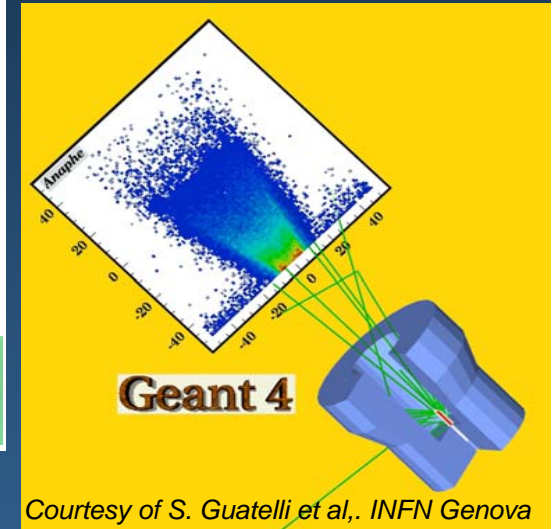
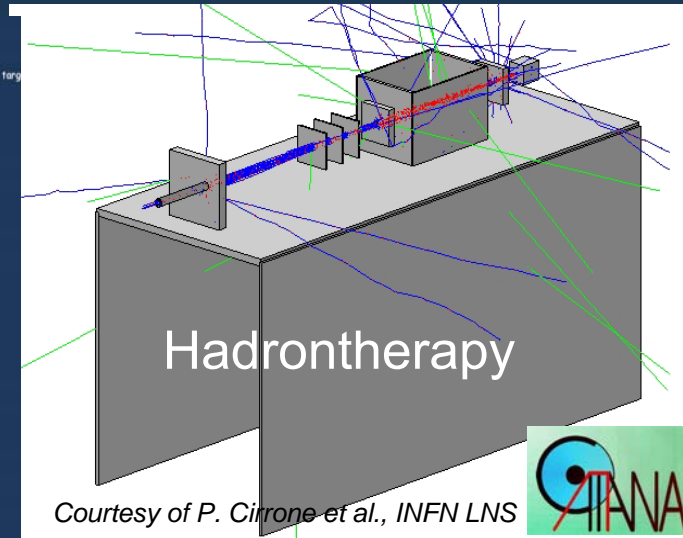
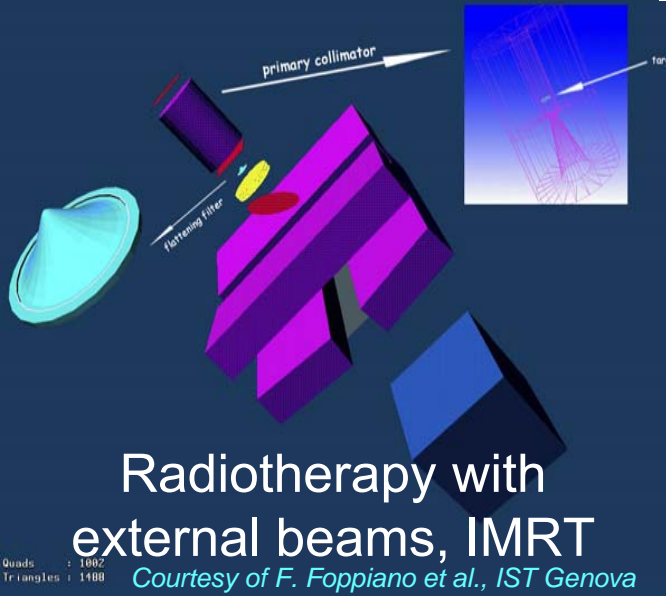
Wide spectrum of physics coverage, variety of physics models

Precise, quantitatively validated physics

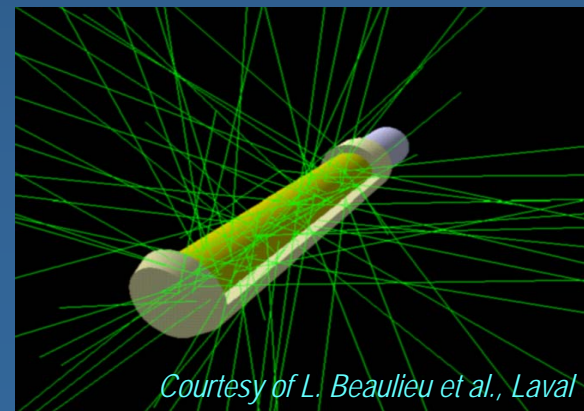
Accurate description of geometry and materials

# Geant 4

# Dosimetry in Medical Applications



## Brachytherapy



# Precise dose calculation

## Geant4 Low Energy Electromagnetic Physics package

- Electrons and photons ( $250/100 \text{ eV} < E < 100 \text{ GeV}$ )
  - Models based on the Livermore libraries (EEDL, EPDL, EADL)
  - Models à la Penelope
- Hadrons and ions
  - Free electron gas + Parameterisations (ICRU49, Ziegler) + Bethe-Bloch
  - Nuclear stopping power, Barkas effect, chemical formula, effective charge etc.
- Atomic relaxation
  - Fluorescence, Auger electron emission, PIXE

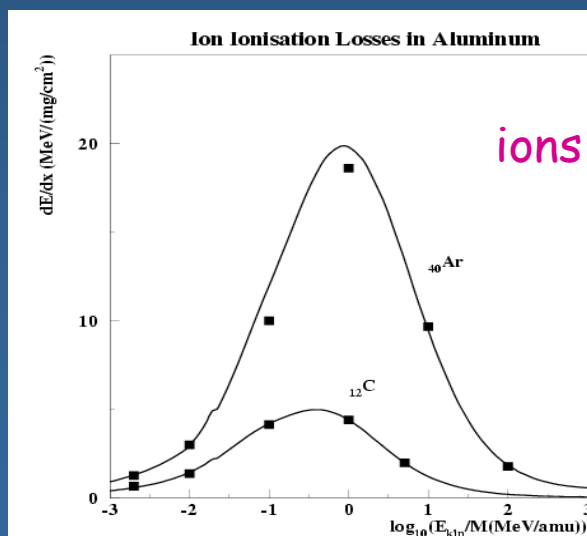
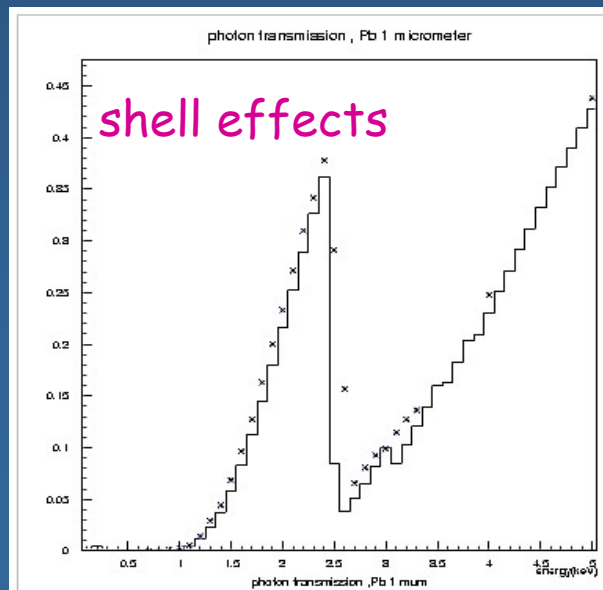
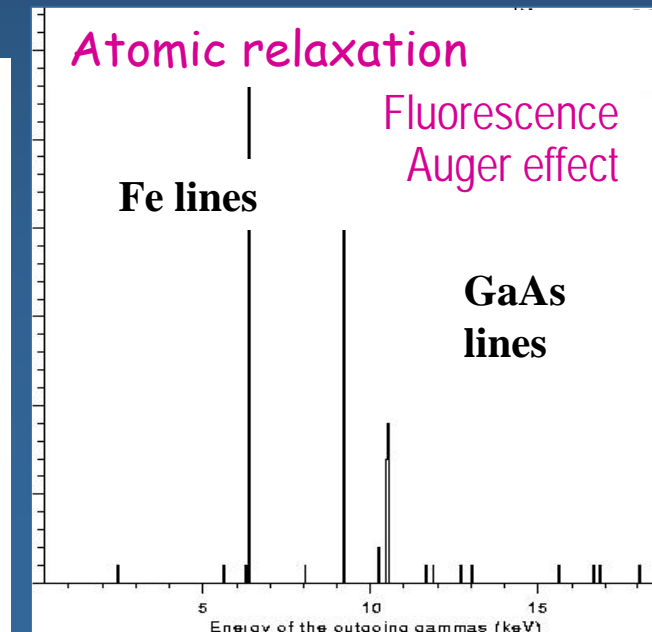


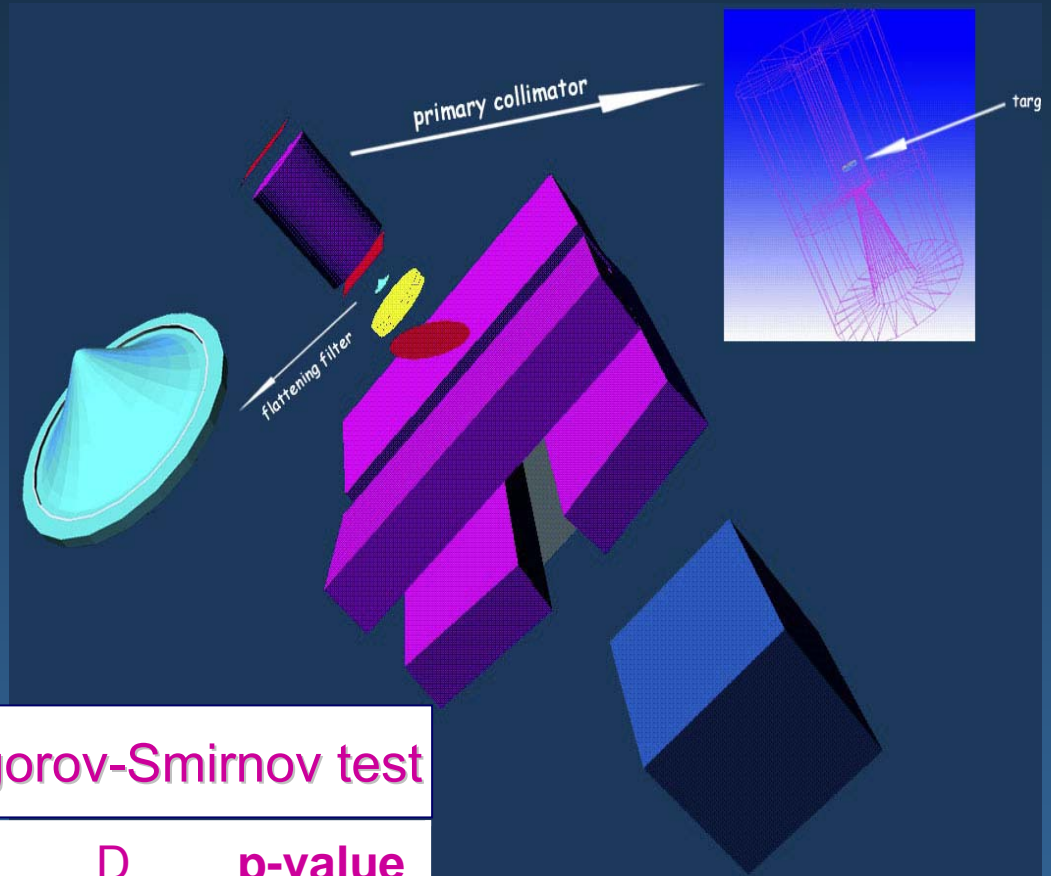
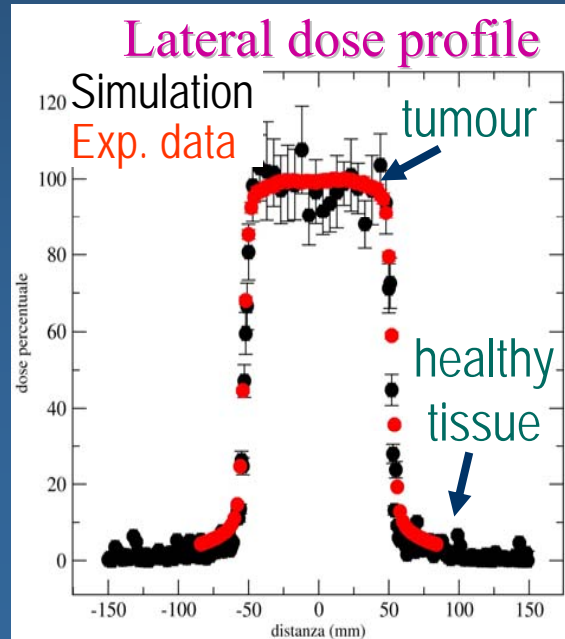
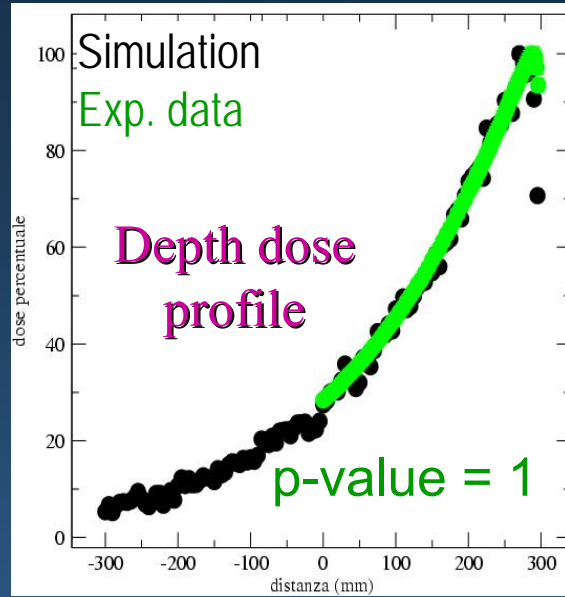
Figure 9: Ion electronic stopping power in aluminum. Points - the best fit on the data from Ref.[12], solid line - GEANT4 parameterisation. The accuracy of the data is about 5%.





# Medical LINAC for IMRT

## Accuracy



### Kolmogorov-Smirnov test

Range	D	p-value
-84 ÷ -60 mm	0.385	<b>0.23</b>
-59 ÷ -48 mm	0.27	<b>0.90</b>
-47 ÷ 47 mm	0.43	<b>0.19</b>
48 ÷ 59 mm	0.30	<b>0.82</b>
60 ÷ 84 mm	0.40	<b>0.10</b>

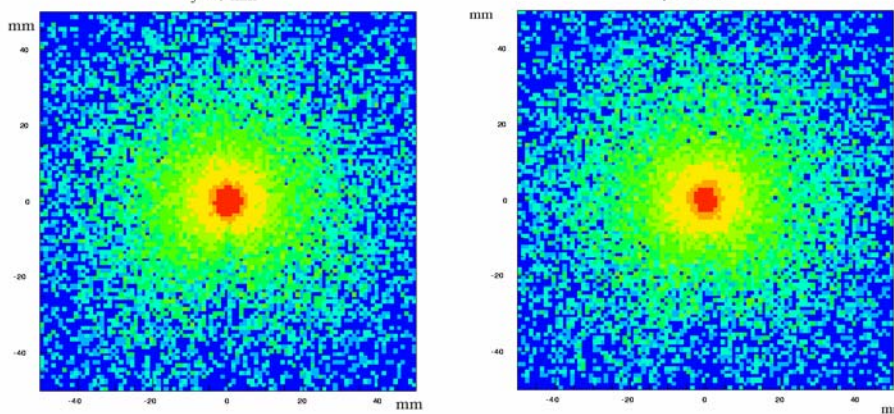


# Flexibility

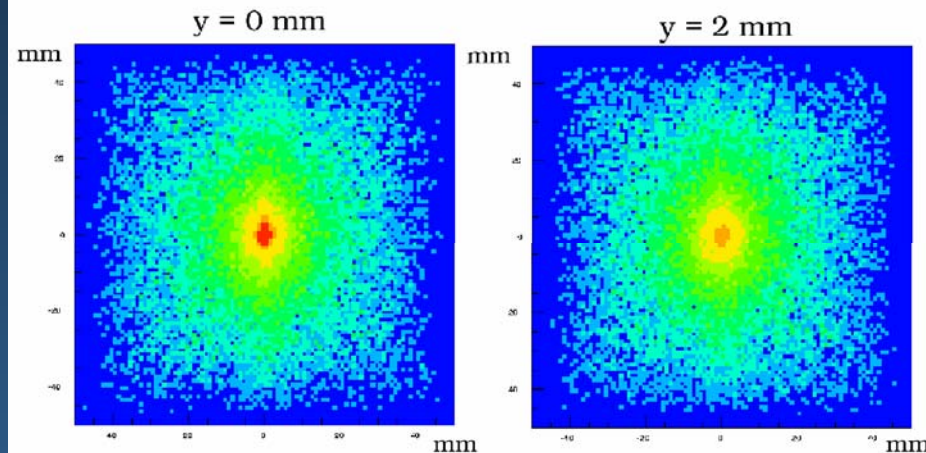
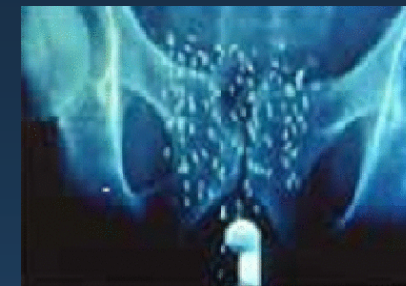
Endocavitary brachytherapy



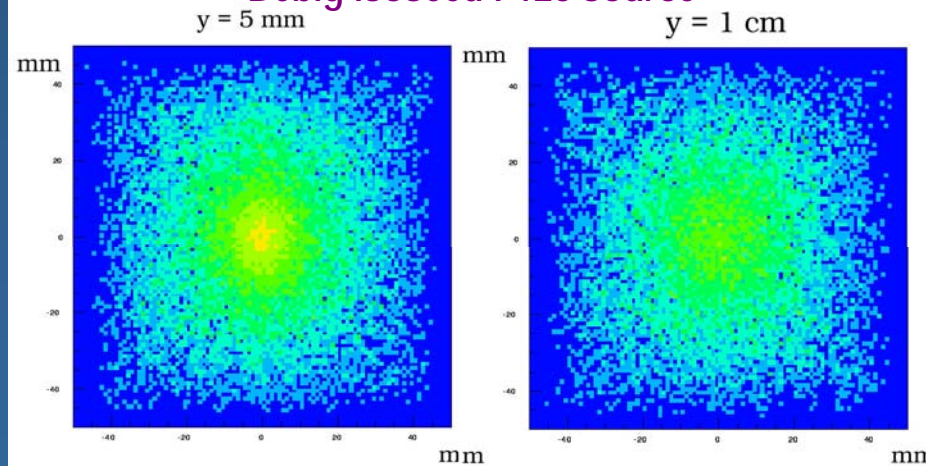
MicroSelectron-HDR source



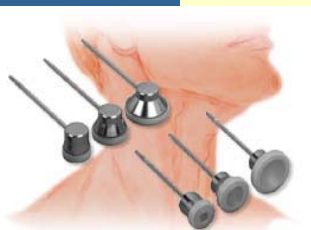
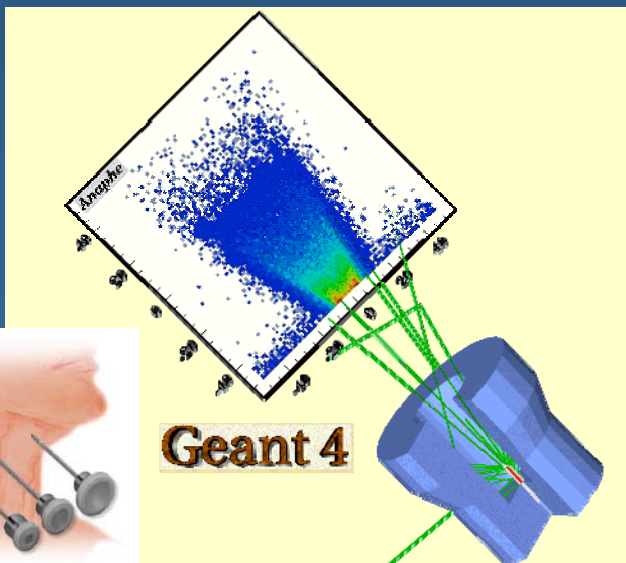
Interstitial brachytherapy



Bebig I-125 source



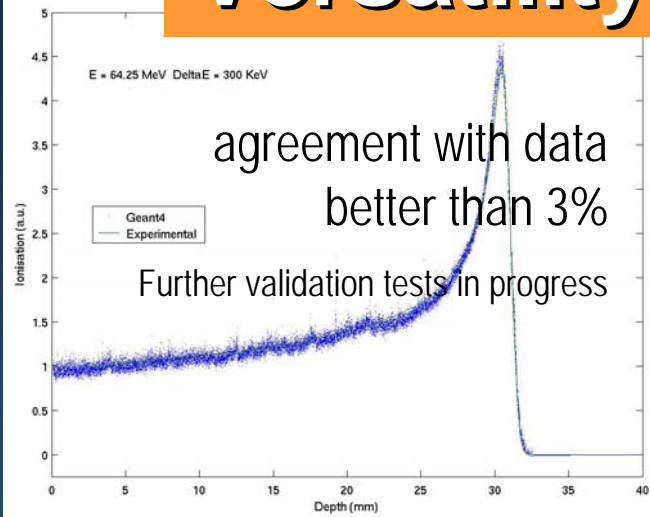
Superficial brachytherapy



# Dosimetry: protons and ions

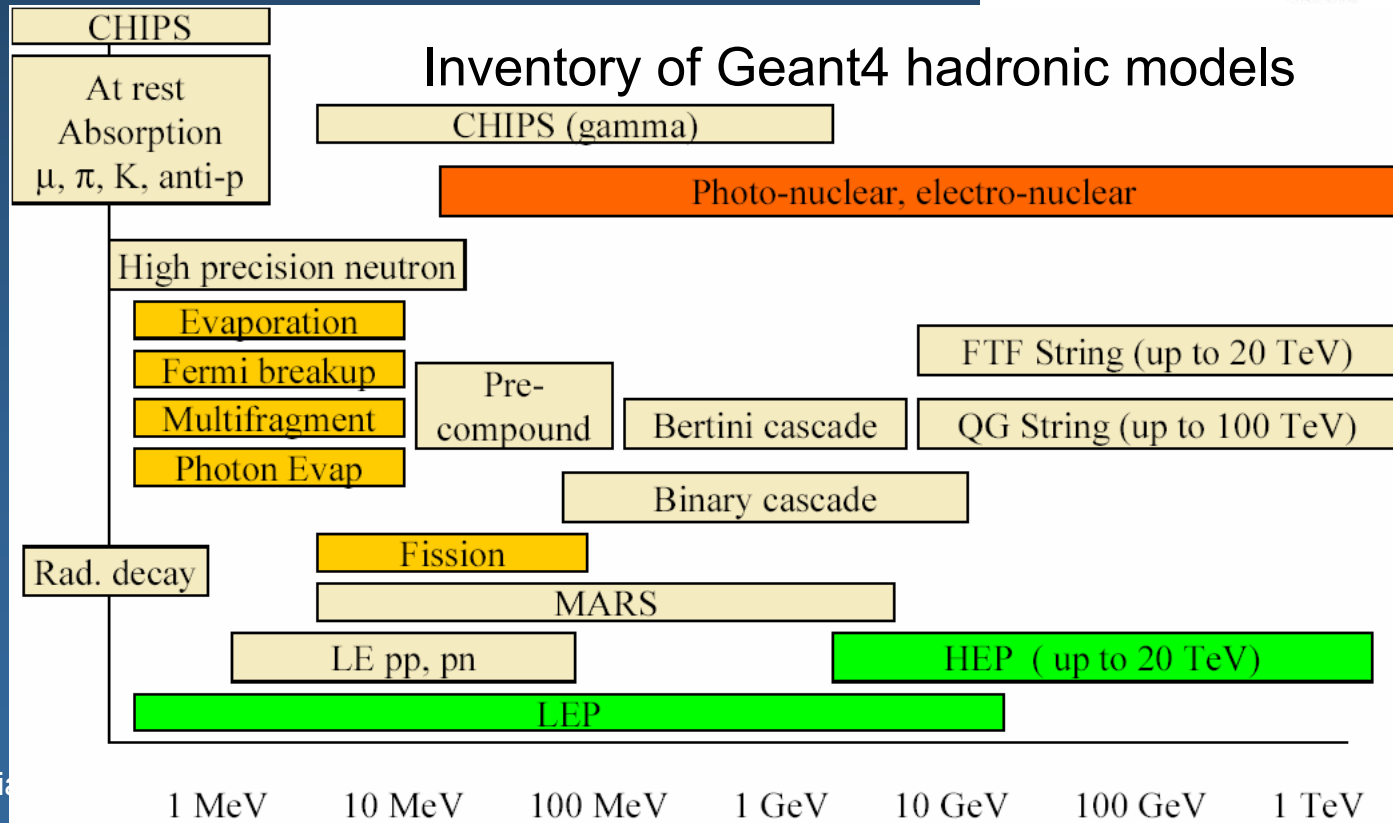
## Versatility

Goodness of Fit	Cramer – von Mises test	Anderson – Darling test
Test statistics	0.06	0.499375
p-value	0.79	0.747452



Electromagnetic only

0.52	0.443831
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# Exotic Geant4 applications...

FAO/IAEA International Conference on  
**Area-Wide Control of Insect Pests:**

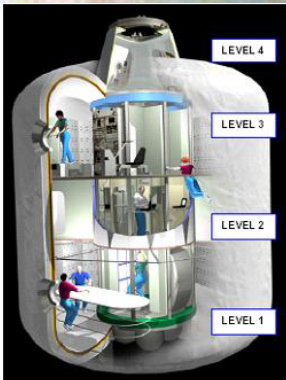
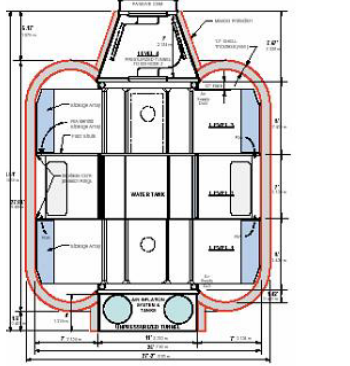
Integrating the Sterile Insect  
and Related Nuclear and Other Techniques

Vienna, May 9-13, 2005

*K. Manai, K. Farah, A.Trabelsi, F. Gharbi and O. Kadri (Tunisia)*

**Dose Distribution and Dose Uniformity in Pupae Treated by  
the Tunisian Gamma Irradiator Using the GEANT4 Toolkit**

# Radiation protection for interplanetary manned missions



Galactic and extra-galactic cosmic rays

Neutrinos

Anomalous cosmic rays

Jovian electrons

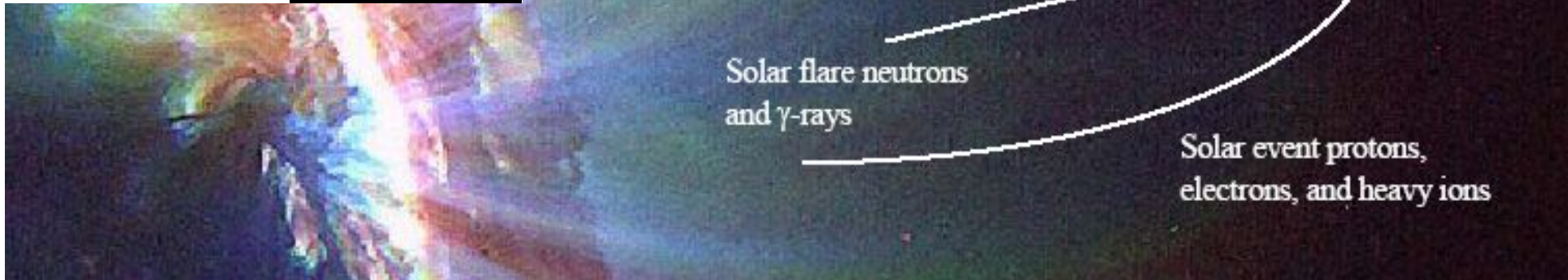
Solar X-rays

Secondary emissions

Solar flare neutrons and  $\gamma$ -rays

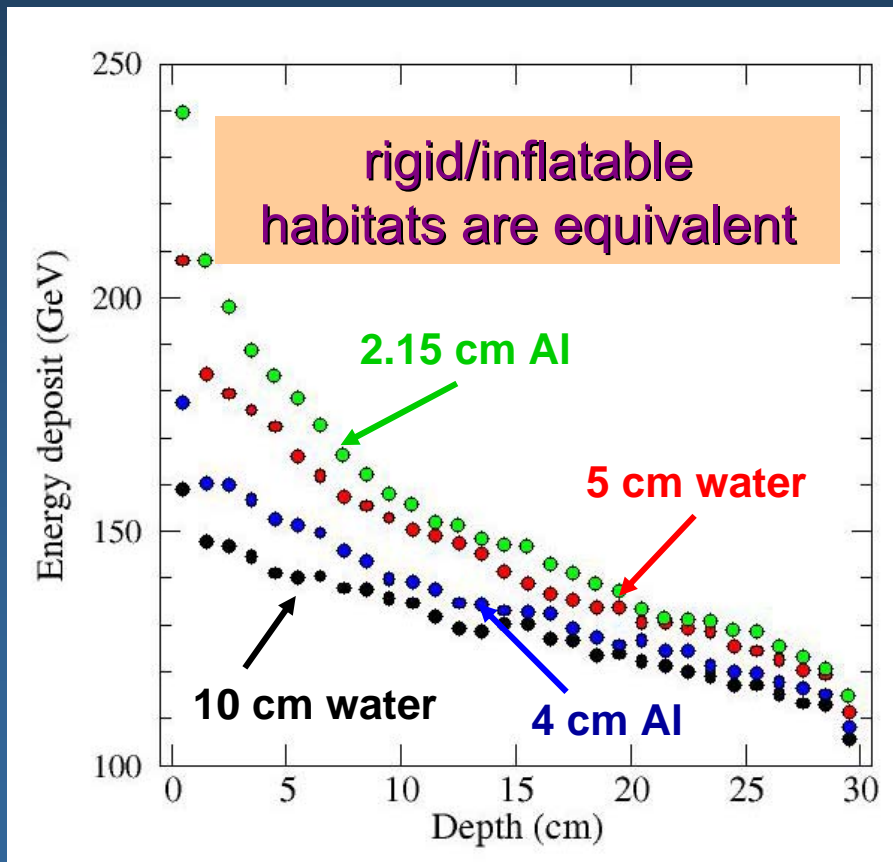
Trapped particles

Solar event protons, electrons, and heavy ions

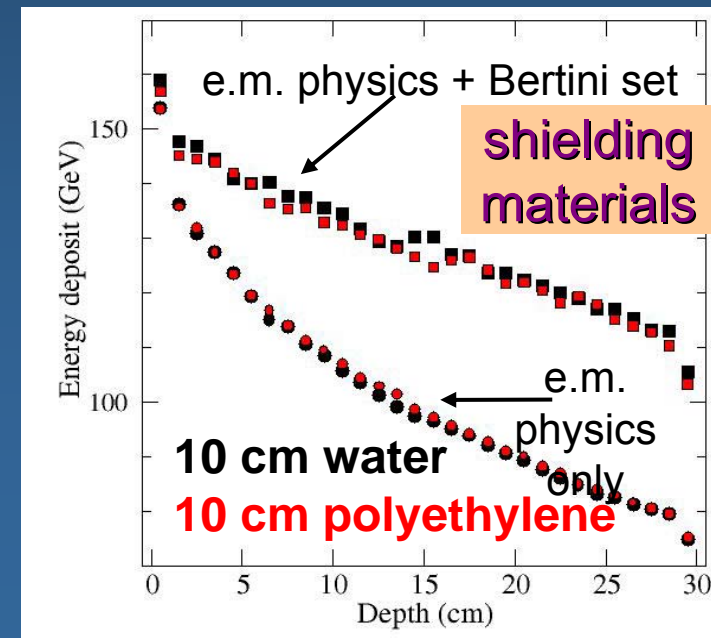
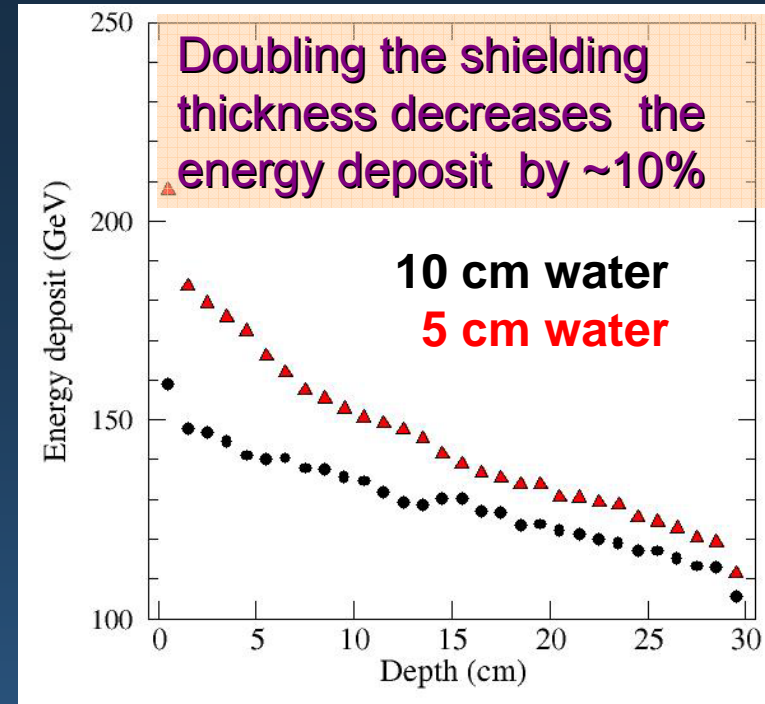


# Geant 4

S. Guatelli et al., Geant4 Simulation for interplanetary manned missions  
Submitted to *IEEE Trans. Nucl. Sci.*



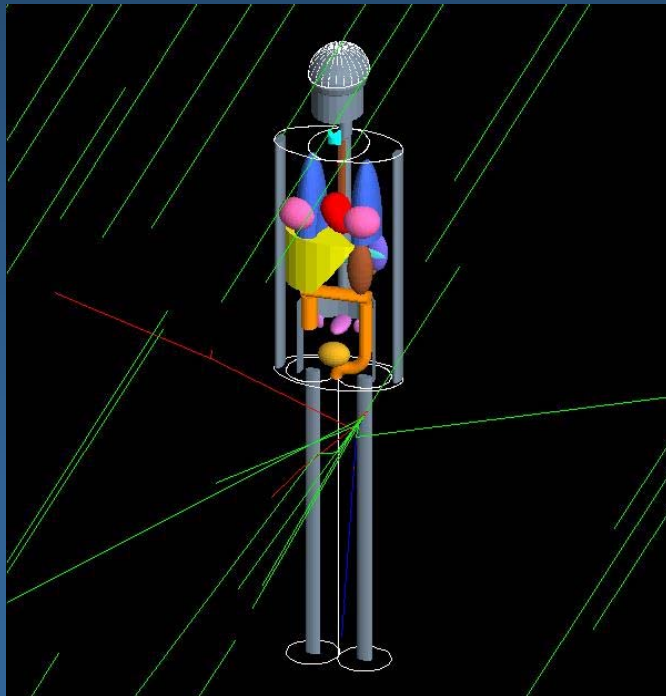
Maria Grazia Pia, *INFN Genova*



A major concern in radiation protection is the  
dose accumulated in organs at risk

# Geant 4

## Anthropomorphic Phantoms



Maria Grazia Pia, *INFN Genova*

- Development of anthropomorphic phantom models for Geant4
  - evaluate dose deposited in critical organs
- Original approach
  - analytical and voxel phantoms in the same simulation environment

Analytical phantoms

Geant4 CSG, BREPS solids

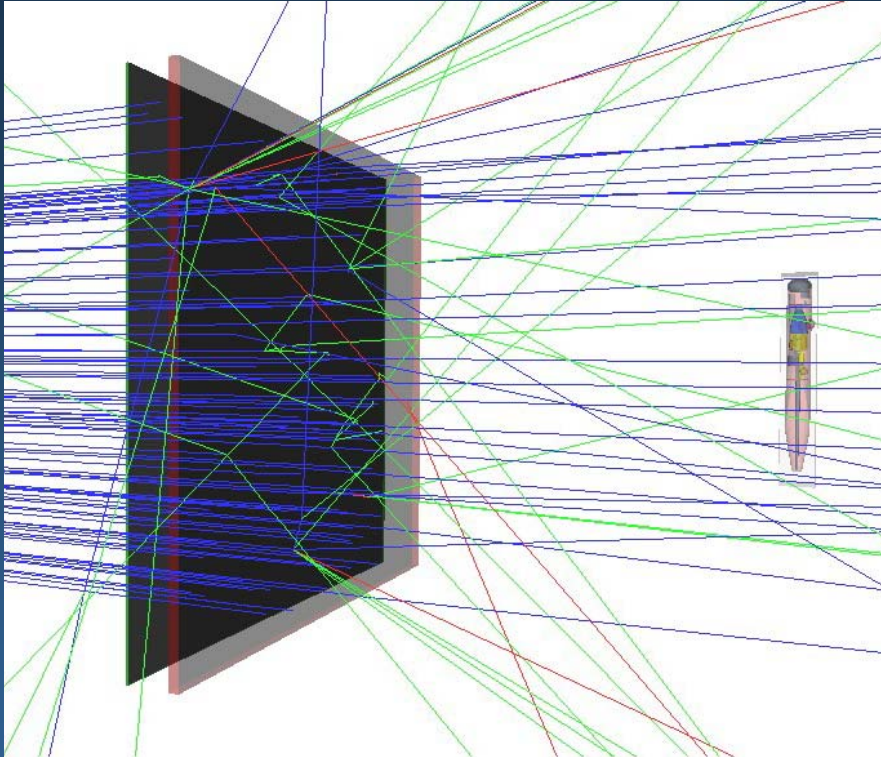
Voxel phantoms

Geant4 parameterised volumes

GDML

for geometry description persistency

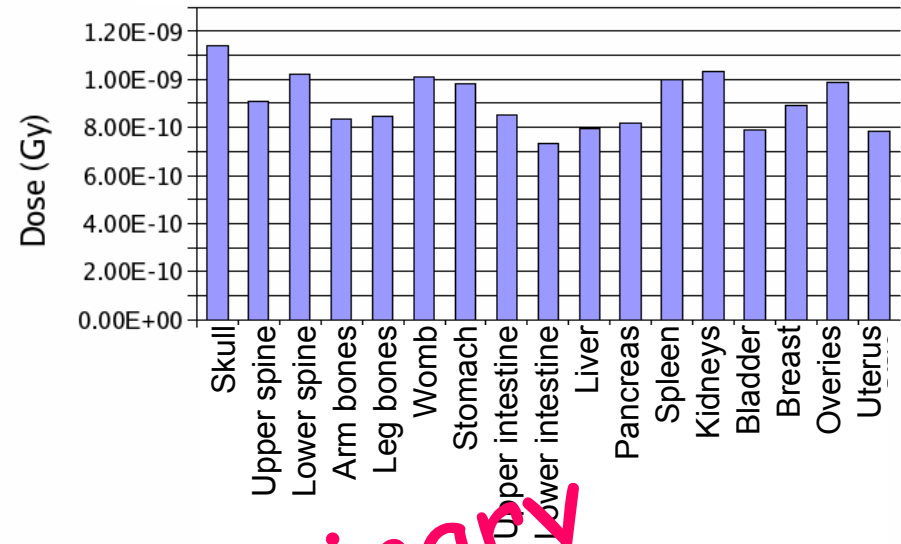
# Radiation exposure of astronauts



Dose calculation in critical organs

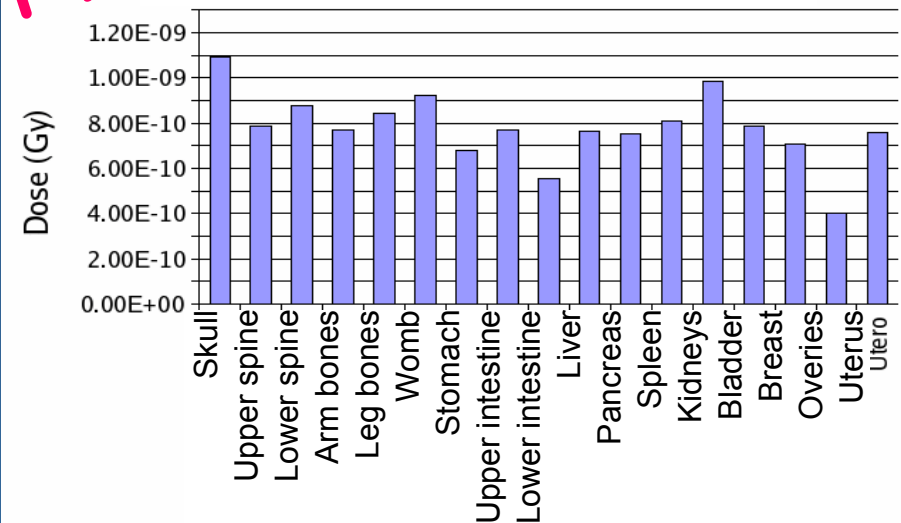
Effects of external shielding  
self-body shielding

5 cm water shielding



Preliminary

10 cm water shielding





# Geant 4

# DNA

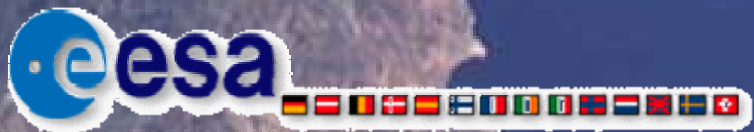
2000/02/27 01:54





Biological models in Geant4

Relevance for space:  
astronaut and aircrew radiation hazards





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

Go Links >>

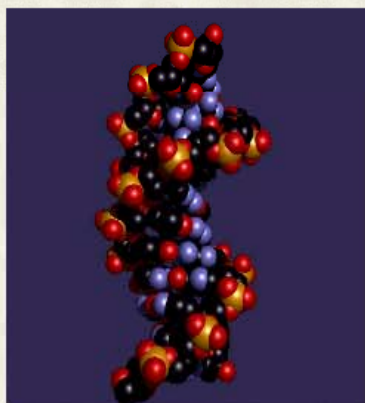


# Geant 4 DNA



- [Home](#)
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- [Documents](#)
- [Talks](#)
- [Papers](#)
- [Meetings](#)
- [Team](#)
  
- [Geant4](#)
- [Geant4-INFN](#)
- [Geant4 LowE Physics](#)
  
- [Useful links](#)

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

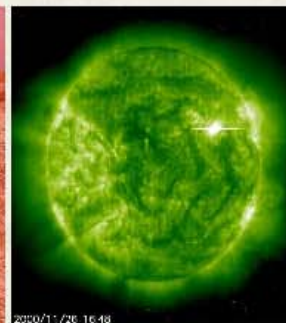


Estimating cancer risk for human exposures to space radiation is a challenge which involves a wide range of knowledge in physics, chemistry, biology and medicine.

Traditionally, the biological effects of radiation are analysed in top-bottom order, i.e. evaluation of the absorbed macroscopic radiation dose at a given location in the biological tissue is translated to the degree of danger it presents, and dose limits are consequently set that are considered to be acceptable.

A novel approach, based on the new-generation object-oriented [Geant4](#) Monte Carlo Toolkit, proceeds in a reverse order, from bottom to top, by analysing the nano-scale effects of energetic particles at the cellular and DNA molecule level.

This project is sponsored by the European Space Agency ([ESA](#)) and is pursued by a multidisciplinary European team of biologists, physicians, physicists, space scientists and software engineers.



Pictures courtesy of ESA

# Geant 4 DNA

International (open) collaboration  
ESA - INFN (*Genova, Torino*) -  
IN2P3 (*CENBG, Univ. Clermont-Ferrand*) - ...

“Sister” activity to  
Geant4 Low-Energy Electromagnetic Physics  
Follows the same rigorous software standards

- **Simulation of nano-scale effects of radiation at the DNA level**
  - Various scientific domains involved  
*medical, biology, genetics, physics, software engineering*
  - Multiple approaches can be implemented with Geant4  
*RBE parameterisation, detailed biochemical processes, etc.*
- **First phase: 2000-2001**
  - Collection of user requirements & first prototypes
- **Second phase: started in 2004**
  - Software development & open source release

# Physics

From the Minutes of LCB (LHCC Computing Board) 21 October, 1997:

“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**.”

# OO technology

## Openness to **extension** and **evolution**

- new implementations can be added w/o changing the existing code

## Robustness and ease of **maintenance**

- **protocols** and well defined dependencies minimize coupling

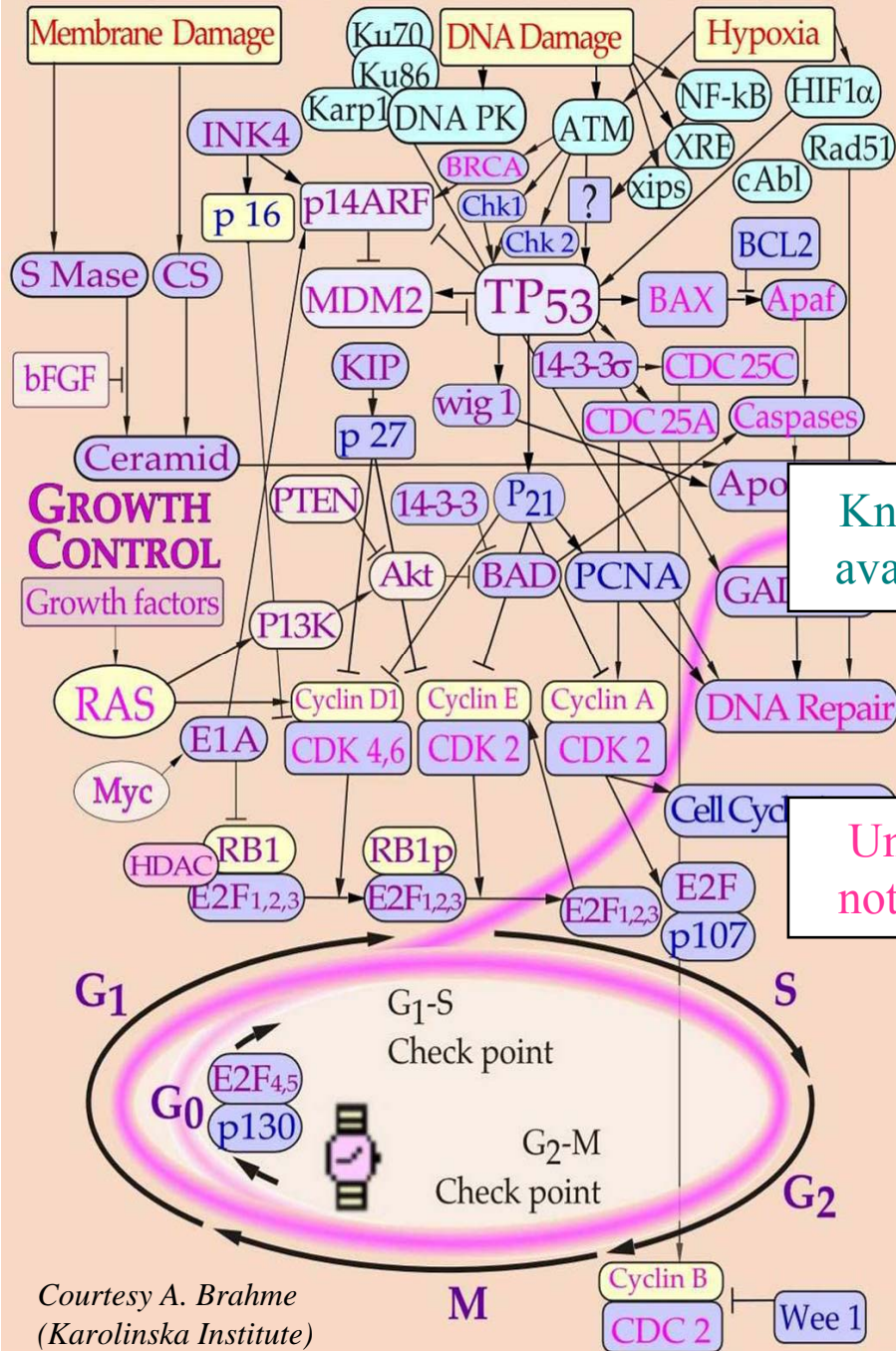
# Strategic vision

# Toolkit

## A set of compatible components

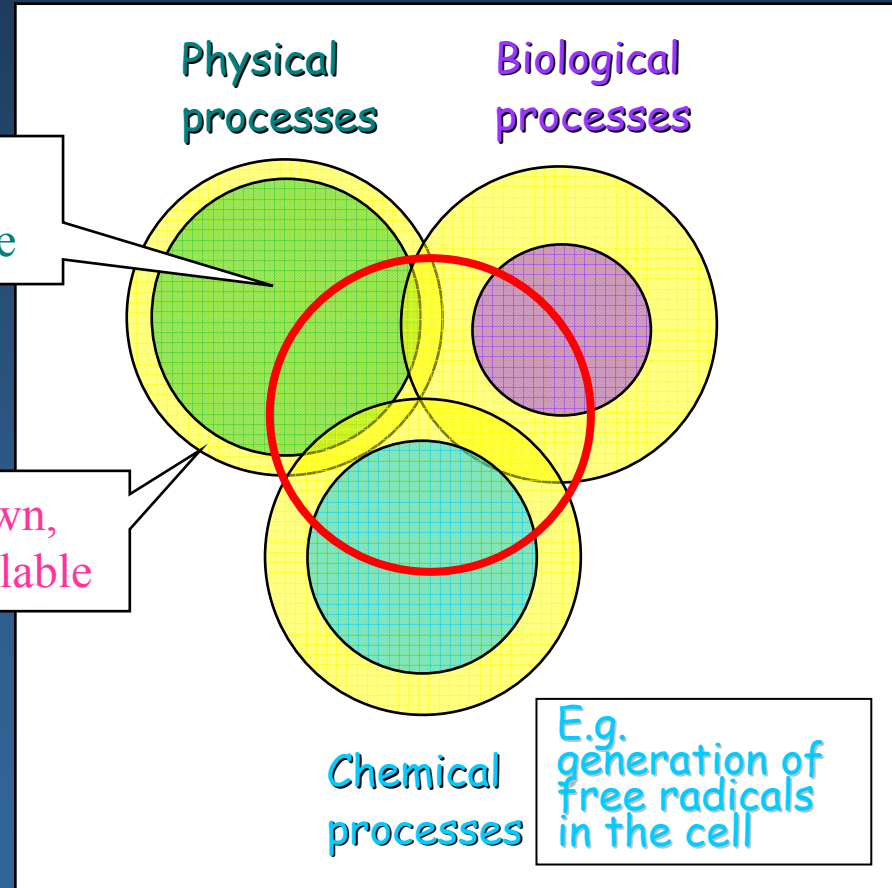
- each component is **specialised** for a specific functionality
- each component can be **refined** independently to a great detail
- components can be **integrated** at any degree of complexity
- it is easy to provide (and use) **alternative** components
- the user application can be **customised** as needed

# DAMAGE AND CELL CYCLE CONTROL



Courtesy A. Brahme  
(Karolinska Institute)

# Biological processes



# Geant 4

## Multiple domains in the same software environment

### ● Macroscopic level

- calculation of dose
- already feasible with Geant4
- develop useful associated tools

### ● Cellular level

- cell modelling
- processes for cell survival, damage etc.

### ● DNA level

- DNA modelling
- physics processes at the eV scale
- bio-chemical processes
- processes for DNA damage, repair etc.

Complexity of  
software, physics and biology  
addressed with an iterative and  
incremental software process



Parallel development  
at all the three levels  
(domain decomposition)



# Theories and models for cell survival

## TARGET THEORY MODELS

- Single-hit model
- Multi-target single-hit model
- Single-target multi-hit model

## MOLECULAR THEORY MODELS

- Theory of radiation action
- Theory of dual radiation action
- Repair-Misrepair model
- Lethal-Potentially lethal model

**Geant 4** approach:  
variety of models all handled  
through the same abstract  
interface

in progress

**Geant 4**

Requirements  
Problem domain analysis

Analysis & Design  
Implementation  
Test

Experimental validation of  
Geant4 simulation models



TARGET THEORY	SINGLE-HIT
TARGET THEORY	MULTI-TARGET SINGLE-HIT
MOLECULAR THEORY	RADIATION ACTION
MOLECULAR THEORY	DUAL RADIATION ACTION
MOLECULAR THEORY	REPAIR-MISREPAIR LIN REP / QUADMIS
MOLECULAR THEORY	REPAIR-MISREPAIR LIN REP / MIS
MOLECULAR THEORY	LETHAL-POTENTIALLY LETHAL
MOLECULAR THEORY	LETHAL-POTENTIALLY LETHAL – LOW DOSE
MOLECULAR THEORY	LETHAL-POTENTIALLY LETHAL – HIGH DOSE
MOLECULAR THEORY	LETHAL-POTENTIALLY LETHAL – LQ APPROX

$$S = e^{-D/D_0}$$

REVISED MODEL

$$S = 1 - (1 - e^{-qD})^n$$

$$S = e^{-q_1 D} [1 - (1 - e^{-q_n D})^n]$$

$$S = e^{-p(\alpha D + \beta D^2)}$$

In progress

$$S = S_0 e^{-k(\xi D + D^2)}$$

$$S = e^{-\alpha D} [1 + (\alpha D T / \epsilon)]^\epsilon$$

$$S = e^{-\alpha D} [1 + (\alpha D / \epsilon)]^{\epsilon \Phi}$$

$$S = \exp\left[-N_{TOT} \left[1 + \frac{N_{PL}}{\epsilon(1 - e^{-\epsilon B A tr})}\right]^\epsilon\right]$$

$$S = e^{-\eta_{AC} D}$$

$$-\ln[S(t)] = (\eta_{AC} + \eta_{AB}) D - \epsilon \ln[1 + (\eta_{AB} D / \epsilon)(1 - e^{-\epsilon B A tr})]$$

$$-\ln[S(t)] = (\eta_{AC} + \eta_{AB} e^{-\epsilon B A tr}) D + (\eta_{AB}^2 / 2\epsilon)(1 - e^{-\epsilon B A tr})^2 D^2$$

# Low Energy Physics extensions

- Specialised processes down to the eV scale
  - at this scale physics processes depend on material, phase etc.
  - in progress: Geant4 processes in water at the eV scale
  - $\beta$ -release: Friday 30 June 2006
- Processes for other material than water to follow
  - interest for radiation effects on components

## Current status

	Electrons	Protons (H <sup>+</sup> )	Hydrogen (H)	Alpha (He <sup>++</sup> )	He <sup>+</sup>	He
Elastic	Brenner (7.5 - 200 eV)	Negligible effect	Negligible effect	Negligible effect	Negligible effect	Negligible effect
	Emfietzoglou (> 200 eV)					
Excitation	Emfietzoglou	Miller and Green	Negligible effect	Miller and Green (1 keV – 15 MeV)	Miller and Green (1 keV – 15 MeV)	Miller and Green (1 keV – 15 MeV)
	Born (7 eV – 10 keV)	Born (100 eV – 10 MeV)				
Charge decrease	Not pertinent to this particle	Dingfelder (100 eV – 2 MeV)	Not pertinent to this particle	In progress	In progress	Not pertinent to this particle
Charge increase	Not pertinent to this particle	Not pertinent to this particle	Miller and Green	Not pertinent to this particle	In progress	In progress
			Dingfelder (0.1 Kev – 100 MeV)			
Ionization	In progress	Rudd (0.1 - 500 keV)	Rudd (0.1 – 100 MeV)	In progress	In progress	In progress
		In progress (> 500 keV)				

# Development process

- **Complex domain**

- physics
- software

- **Collaboration with theorists**

- **Innovative design introduced in Geant4**

- Policy-based class design
- Parameterised classes: policies are cross section models, models for final state calculation etc.
- Flexibility of modelling + performance optimisation

- **Collaboration with experimentalists for model validation**

- Geant4 physics validation at low energies is difficult!

## Cross sections

	Electrons	Protons (H+)	Hydrogen (H)	Alpha (He++)	He+	He
Elastic	Brenner (7.5 - 200 eV)	Negligible effect	Negligible effect	Negligible effect	Negligible effect	Negligible effect
	Emfietzoglou (> 200 eV)					
Excitation	Emfietzoglou	Miller and Green	Negligible effect	Miller and Green (1 keV – 15 MeV)	Miller and Green (1 keV – 15 MeV)	Miller and Green (1 keV – 15 MeV)
	Born (7 eV – 10 keV)	Born (100 eV – 10 MeV)				
Charge decrease	Process not pertinent to this particle	Dingfelder (100 eV – 2 MeV)	Process not pertinent to this particle	In progress	In progress	Process not pertinent to this particle
Charge increase	Process not pertinent to this particle	Process not pertinent to this particle	Miller and Green Dingfelder (0.1 Kev – 100 MeV)	Process not pertinent to this particle	In progress	In progress
Ionization	In progress	Rudd (0.1 - 500 keV)	Rudd (0.1 – 100 MeV)	In progress	In progress	In progress
		In progress (> 500 keV)				

## Process kinematics

	Electrons	Protons (H+)	Hydrogen (H)	Alpha (He++)	He+	He
Elastic	Brenner (7.5 - 200 eV)	Negligible effect	Negligible effect	Negligible effect	Negligible effect	Negligible effect
	Emfietzoglou (> 200 eV)					
Excitation	Emfietzoglou	Miller and Green	Negligible effect	Miller and Green (1 keV – 15 MeV)	Miller and Green (1 keV – 15 MeV)	Miller and Green (1 keV – 15 MeV)
	Born (7 eV – 10 keV)	Born (100 eV – 10 MeV)				
Charge decrease	Process not pertinent to this particle	Dingfelder (100 eV – 2 MeV)	Process not pertinent to this particle	In progress	In progress	Process not pertinent to this particle
Charge increase	Process not pertinent to this particle	Process not pertinent to this particle	Miller and Green Dingfelder (0.1 Kev – 100 MeV)	Process not pertinent to this particle	In progress	In progress
Ionization	In progress	Rudd (0.1 - 500 keV)	Rudd (0.1 – 100 MeV)	In progress	In progress	In progress
		In progress (> 500 keV)				

## Final state generation

	Electrons	Protons (H+)	Hydrogen (H)	Alpha (He++)	He+	He
Elastic	Brenner (7.5 - 200 eV)	Negligible effect	Negligible effect	Negligible effect	Negligible effect	Negligible effect
	Emfietzoglou (> 200 eV)					
Excitation	Emfietzoglou	Miller and Green	Negligible effect	Miller and Green (1 keV – 15 MeV)	Miller and Green (1 keV – 15 MeV)	Miller and Green (1 keV – 15 MeV)
	Born (7 eV – 10 keV)	Born (100 eV – 10 MeV)				
Charge decrease	Process not pertinent to this particle	Dingfelder (100 eV – 2 MeV)	Process not pertinent to this particle	In progress	In progress	Process not pertinent to this particle
Charge increase	Process not pertinent to this particle	Process not pertinent to this particle	Miller and Green Dingfelder (0.1 Kev – 100 MeV)	Process not pertinent to this particle	In progress	In progress
Ionization	In progress	Rudd (0.1 - 500 keV)	Rudd (0.1 – 100 MeV)	In progress	In progress	In progress
		In progress (> 500 keV)				

# Why these models?

## ● No emotional attachment to any of the models

- **Toolkit:** offer a wide choice among many available alternatives
- Complementary models
- No “one size fits all”

## ● Powerful design

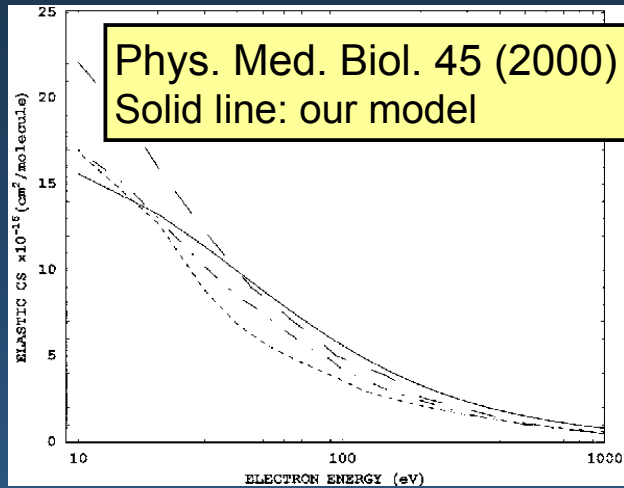
- Abstract interfaces: the kernel is blind to any specific modelling
- Specialization of processes through template instantiation
- Transparency of policy implementation
  - *e.g.: cross sections may be from analytical models or from experimental data*
- Open proliferation of processes, policies and their instantiations

## ● Improvements, extensions, options

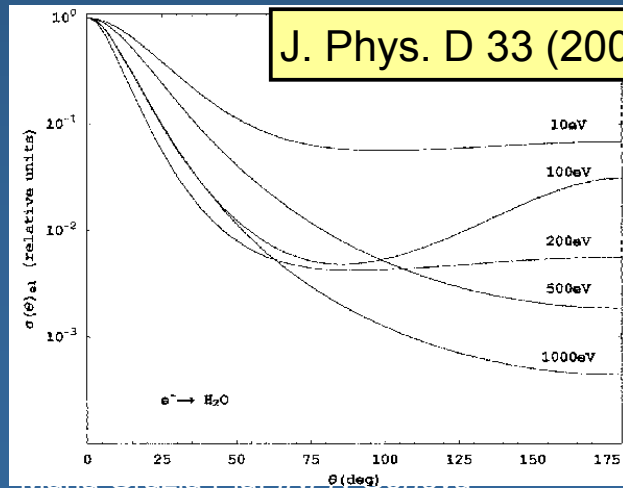
- Open
- Collaboration is welcome (experimental/modelling/software)
- Sound software engineering

# Elastic scattering

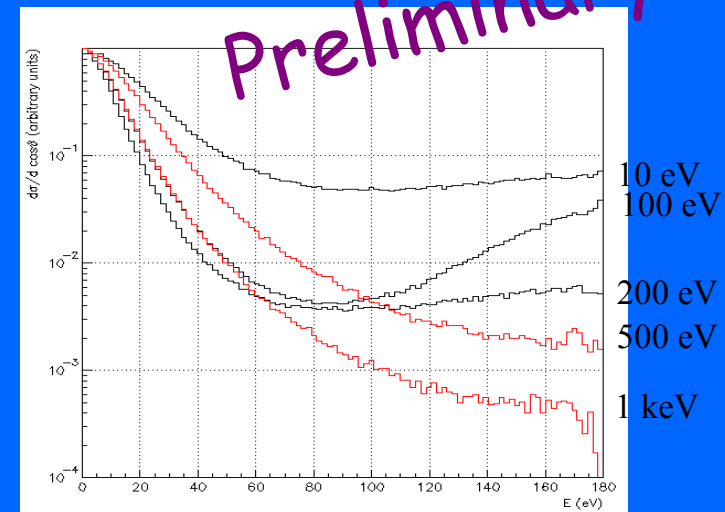
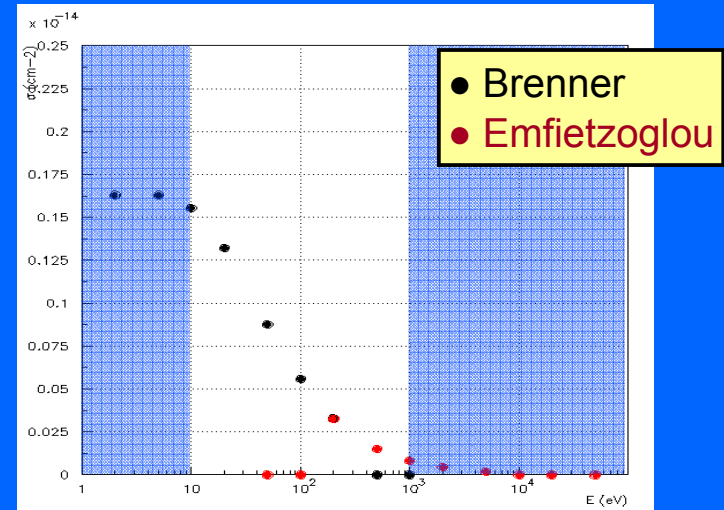
## Total cross section



## Angular distribution

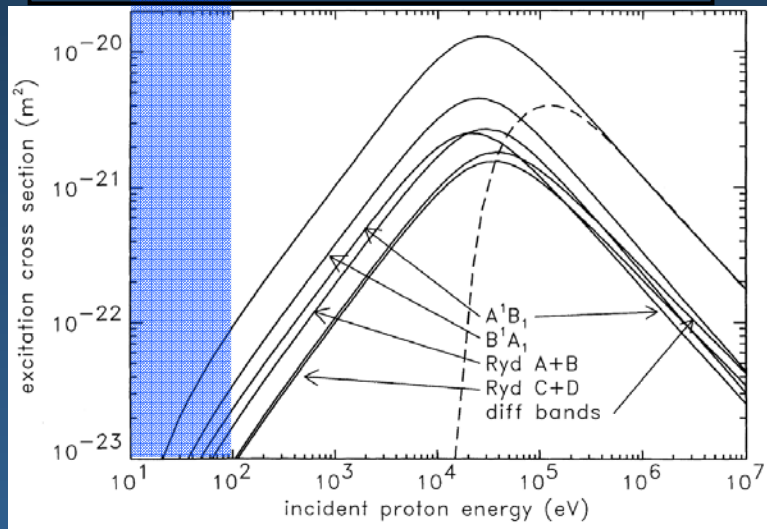


# Geant 4



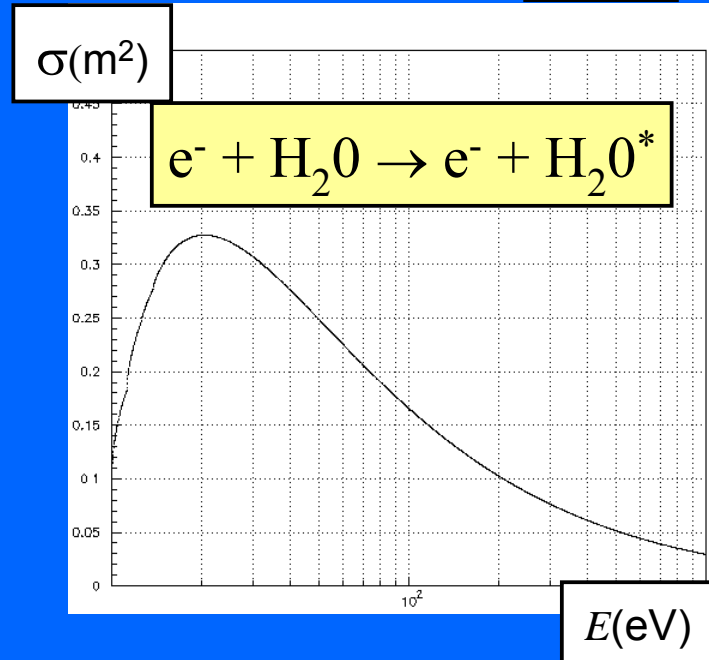
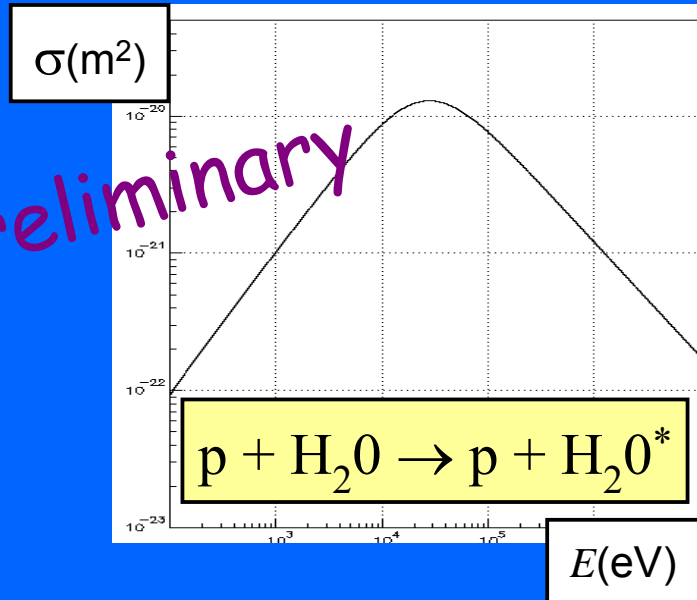
# Excitation

Rad. Phys. Chem. 59 (2000) 255-275



# Geant 4

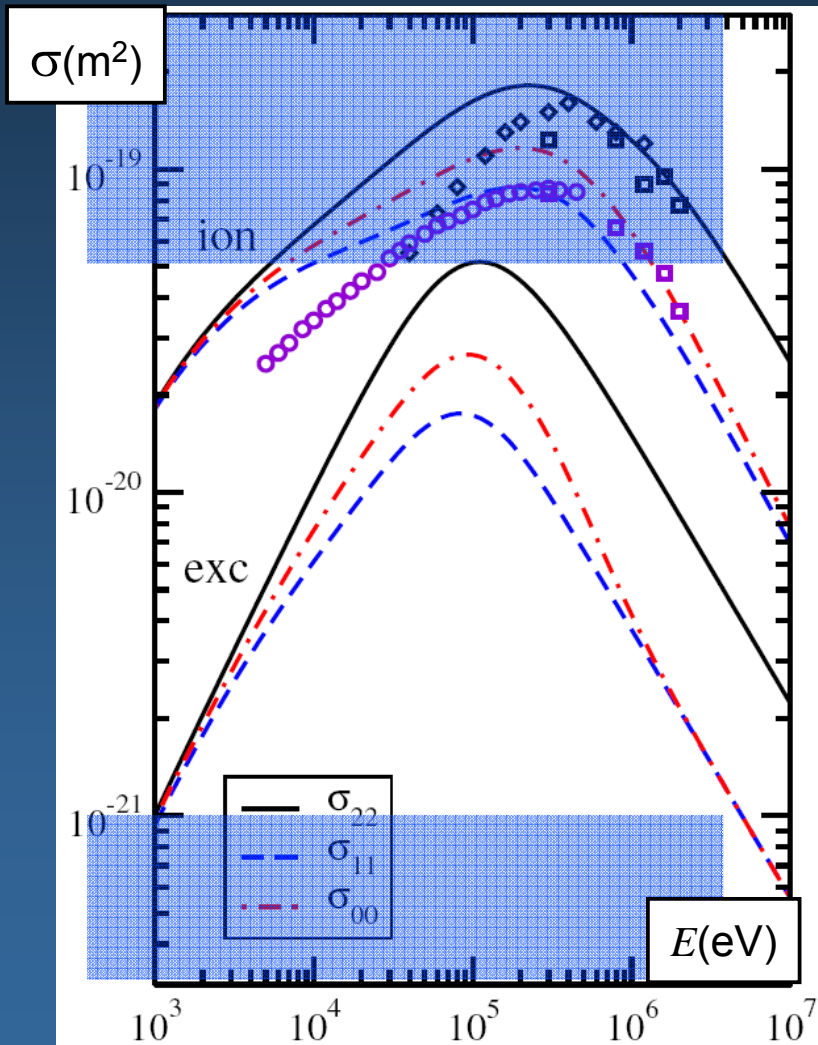
Preliminary





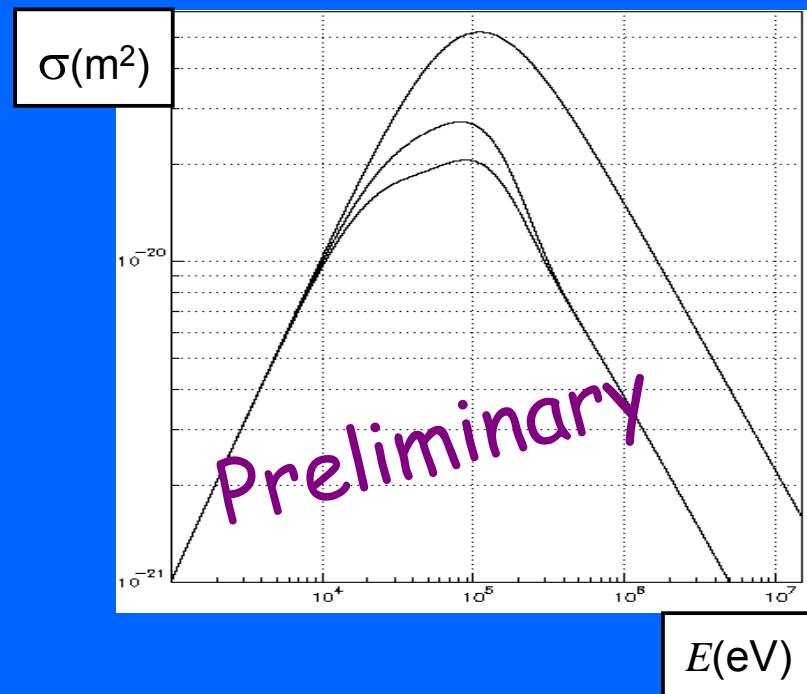
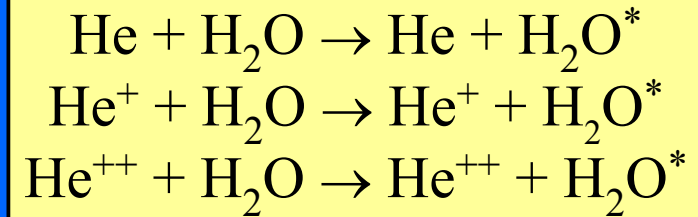
# Excitation

Rad. Phys. Chem. 59 (2000) 255-275

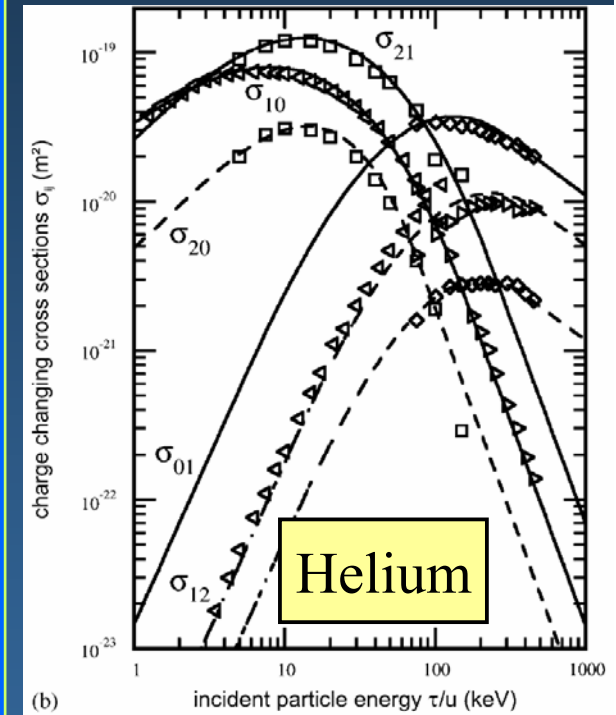
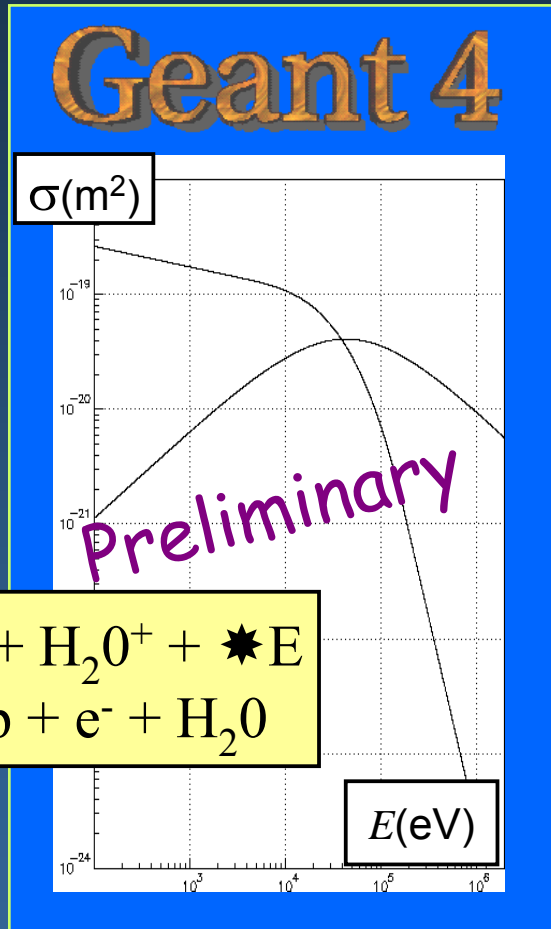
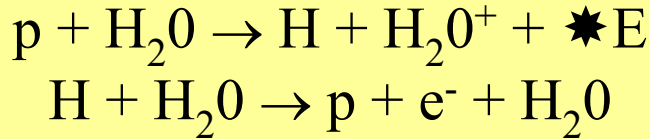
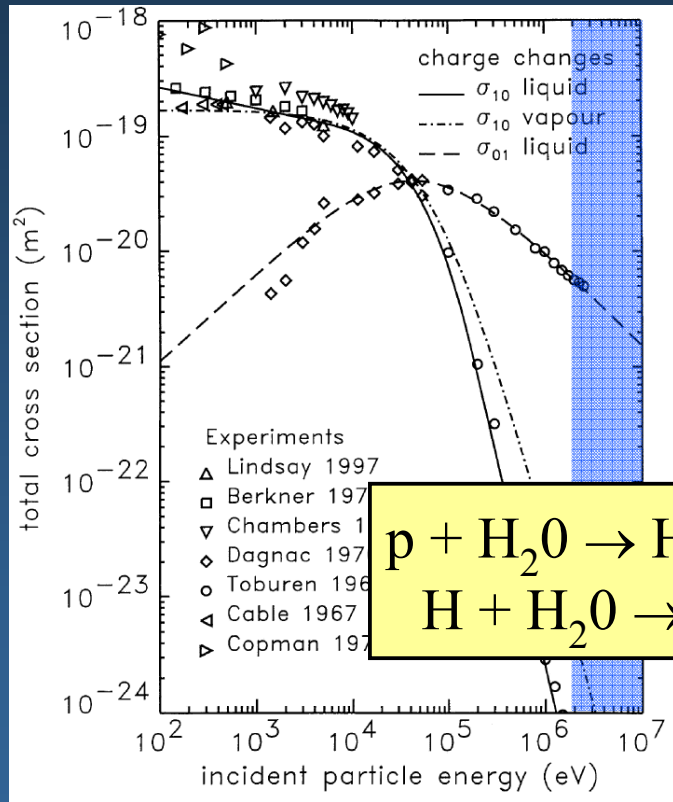


Maria Grazia Pia, INFN Genova

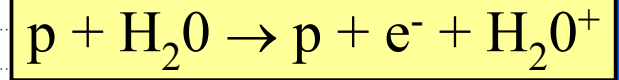
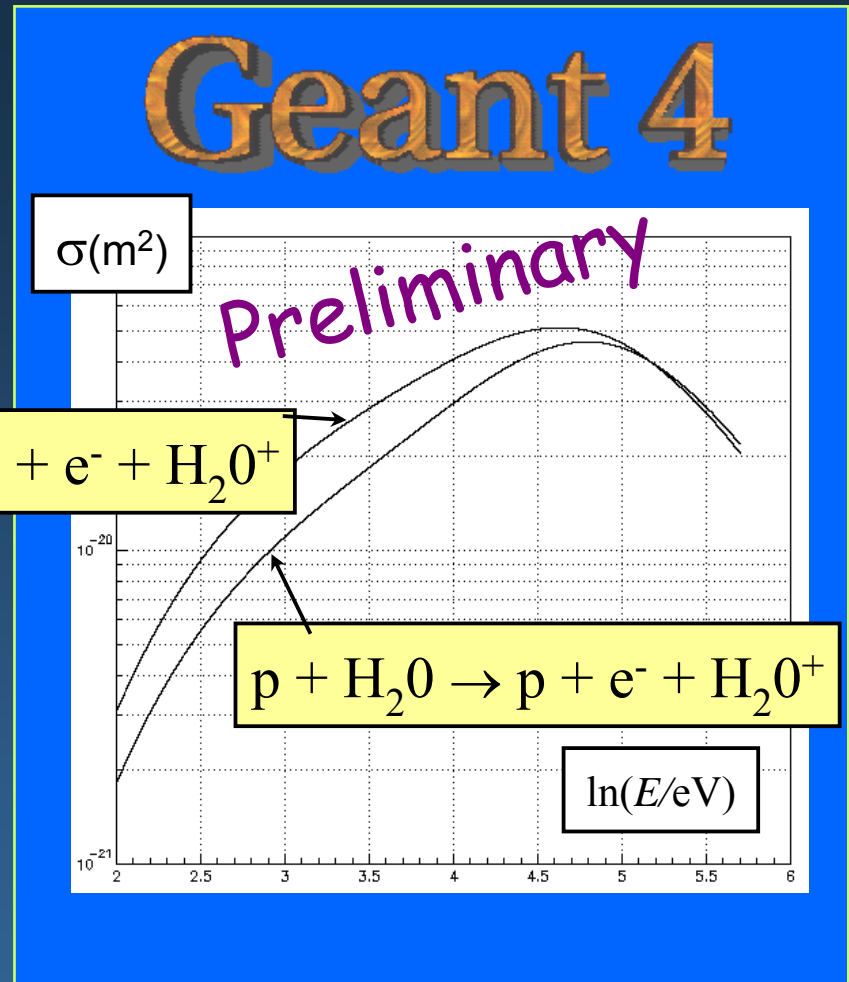
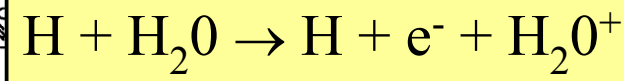
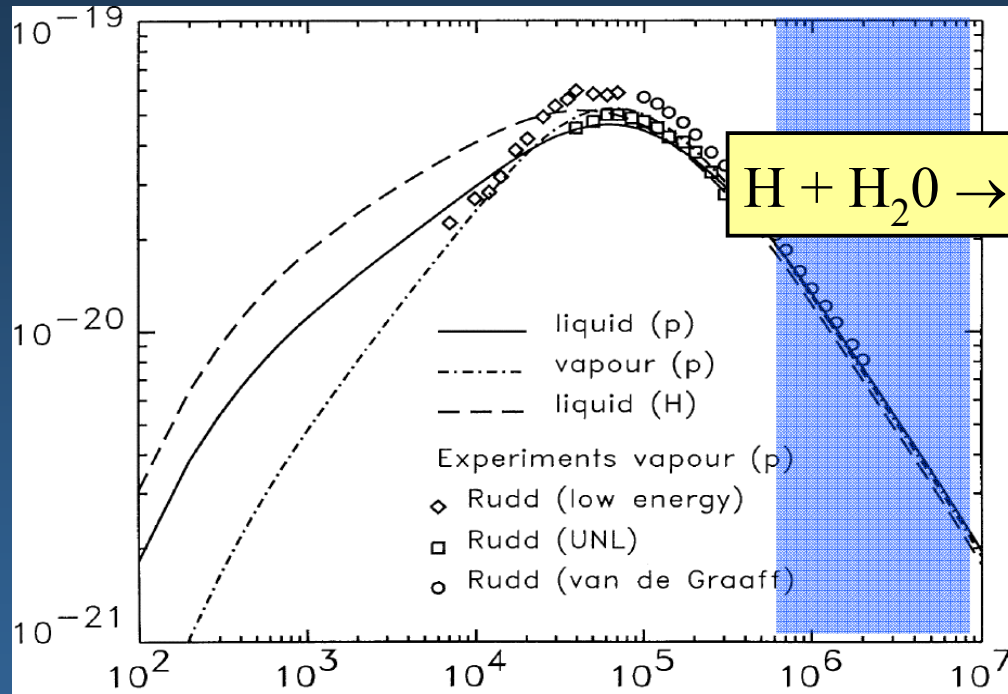
# Geant 4



# Charge transfer



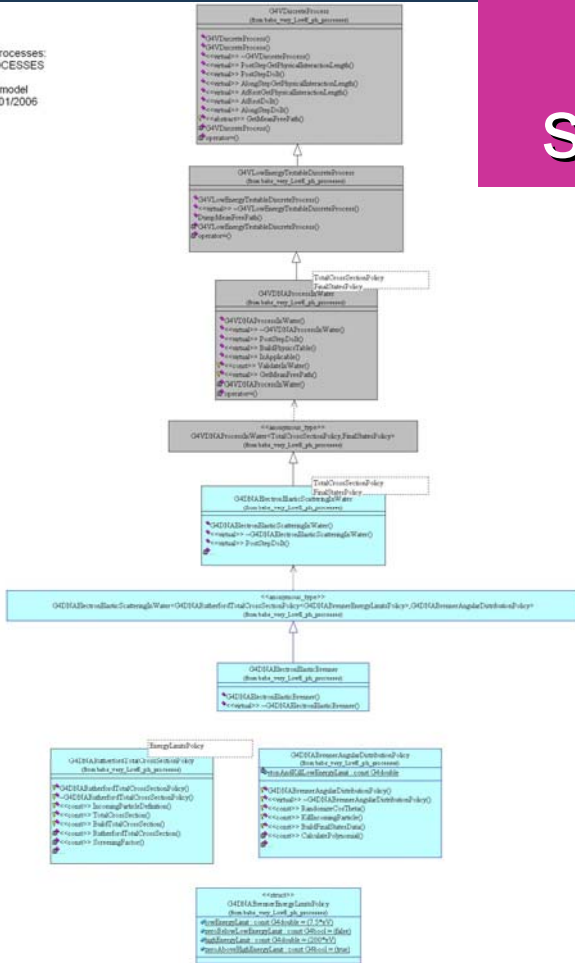
# Ionisation



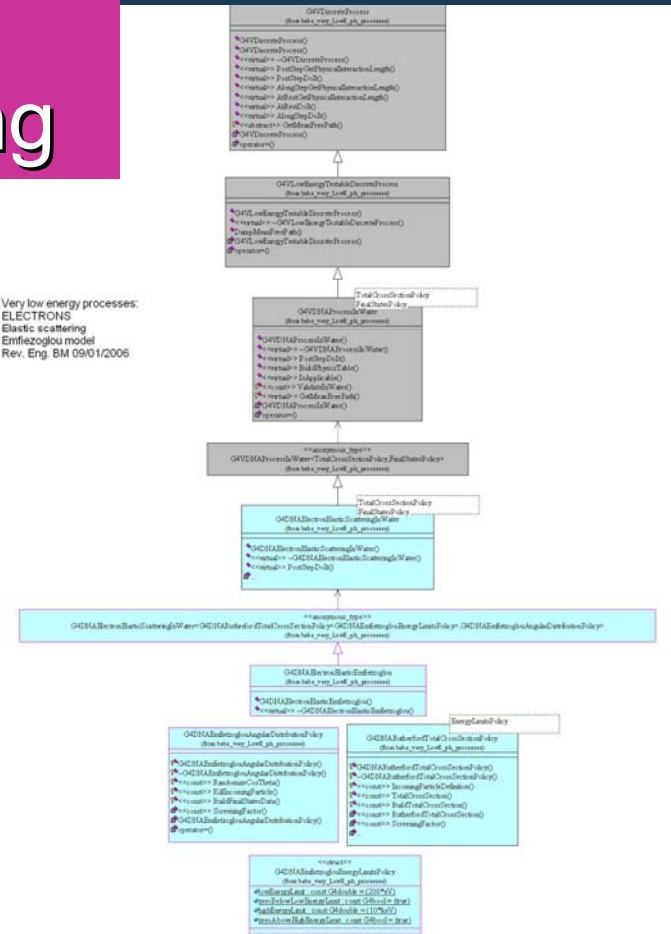
# What is behind...

## Elastic scattering

Very low energy processes:  
ELECTRON PROCESSES  
Elastic scattering  
Brenner & Zaidler model  
Rev. Eng. BM 09/01/2006



Very low energy processes:  
ELECTRONS  
Elastic scattering  
Emfiezoglou model  
Rev. Eng. BM 09/01/2006



...and more

## Excitation

**Policy based classes are parameterised classes**  
*(classes that use other classes as a parameter)*

Advantage w.r.t. a conventional strategy pattern:  
policies are not required to inherit from a base class

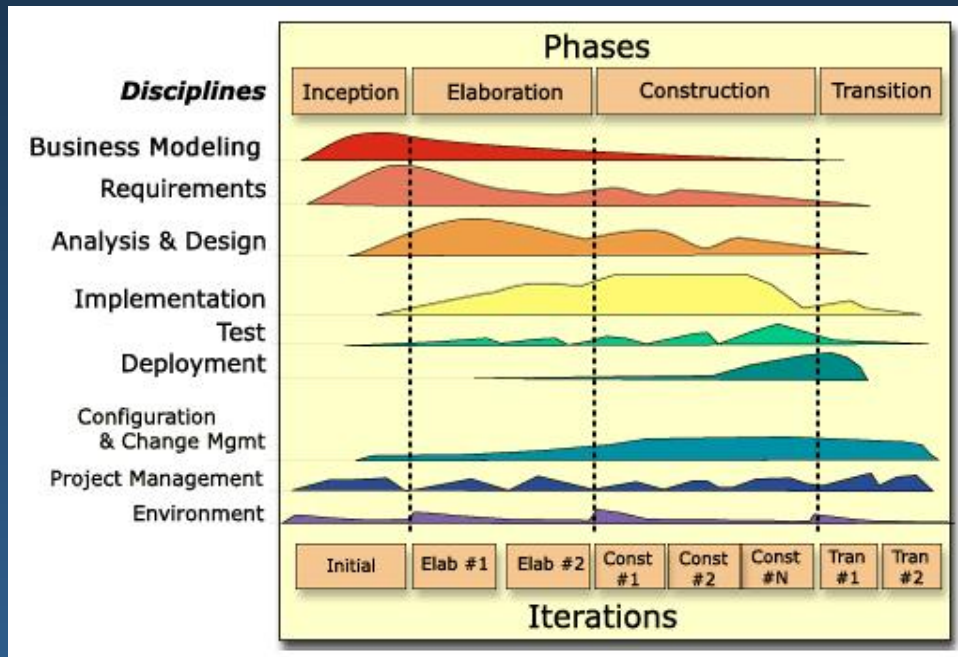
This means a **weaker dependency** of the policy and  
the policy based class on the policy interface

In complex situations this makes a design  
**more flexible and open to extension**

The code is **bound at compilation time**  
No need of virtual methods, resulting in **faster execution**

**Rigorous software engineering**  
**Sophisticated design based on advanced technology**

# ...and behind everything



## Unified Process



## A rigorous software process

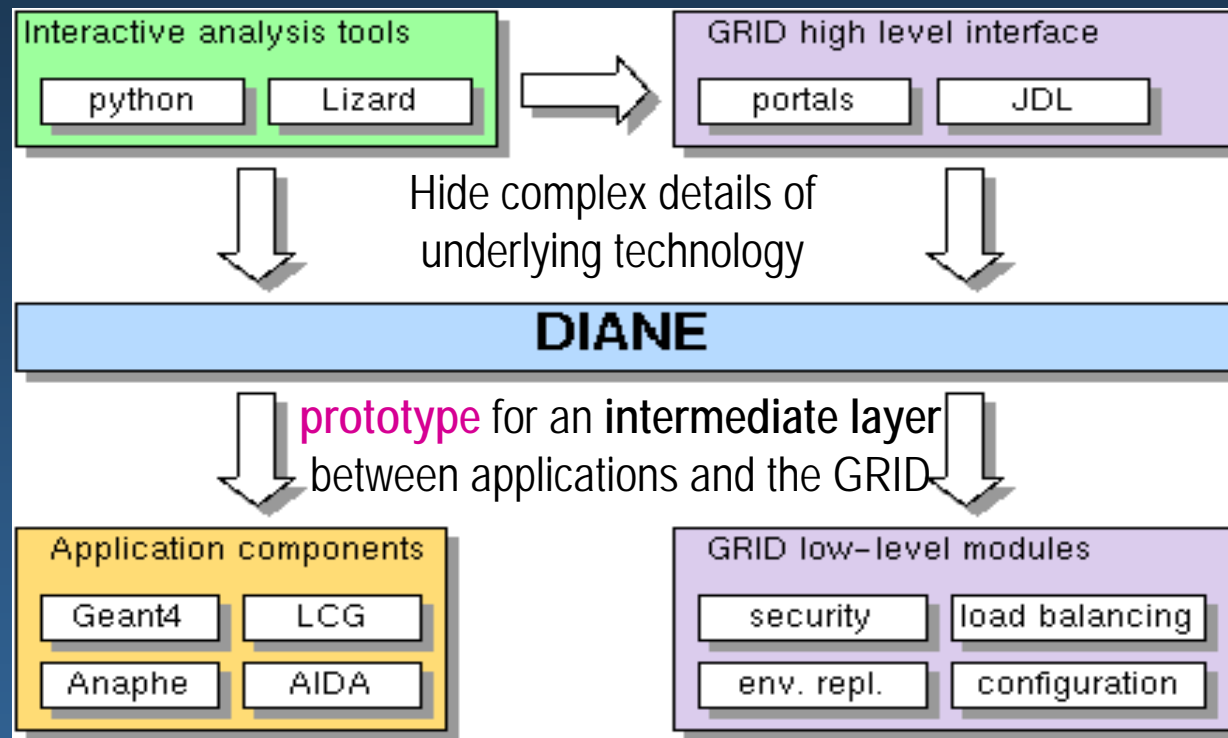
Incremental and iterative lifecycle

RUP™ as process framework, tailored to the specific project

Mapped onto ISO 15504

# Distributed computing environment

Speed of execution is a concern for a simulation at a micro/nano-scale



## DIANE

Distributed Analysis Environment

Developed by  
J. Moscicki, CERN/IT

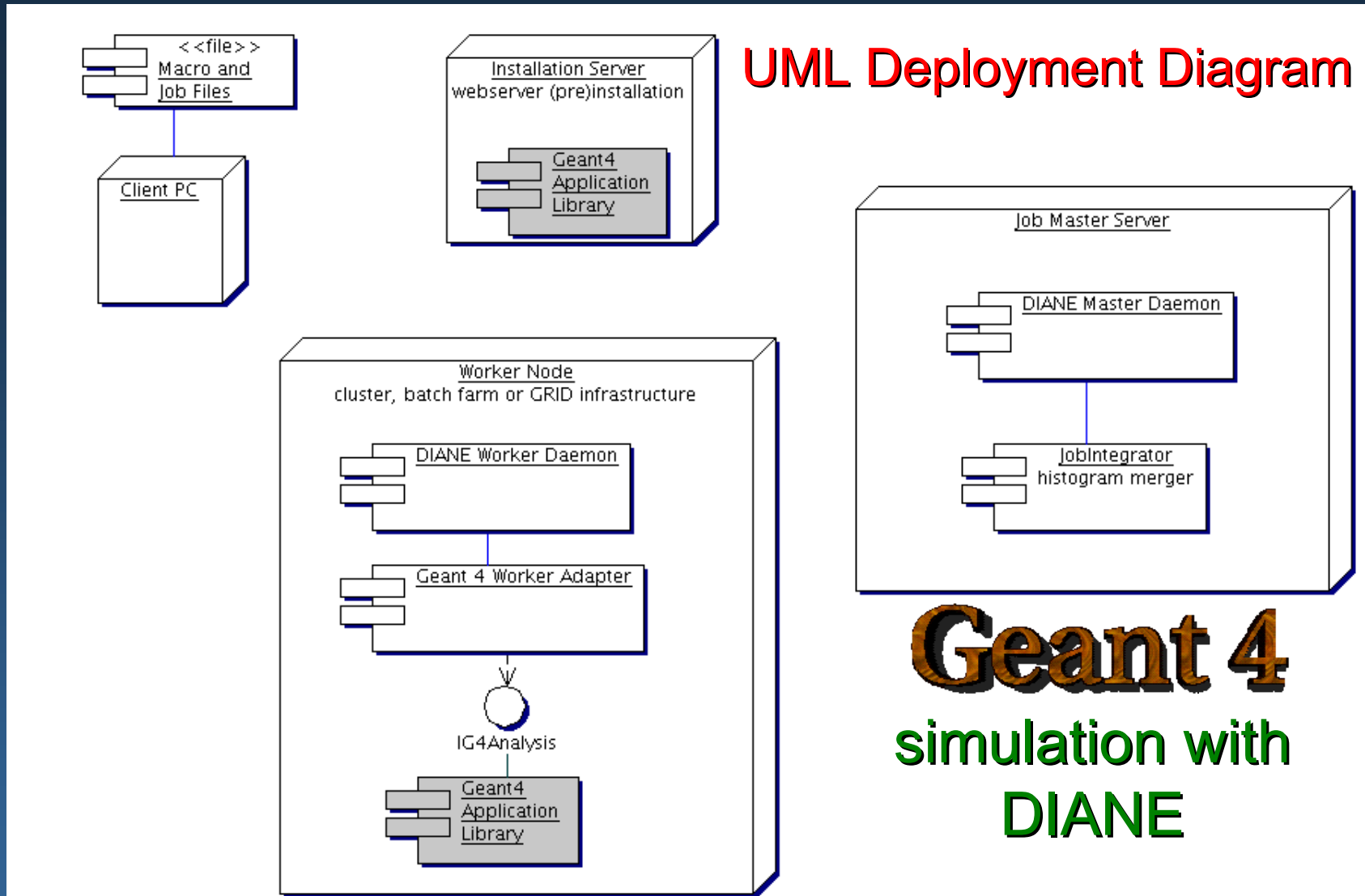
<http://cern.ch/DIANE>

**Master-Worker**  
architectural pattern

## Parallel cluster processing

- Transparent execution on a local farm or on a grid
- Easy access to underlying GRID technology
- Application independent

# UML Deployment Diagram



**Geant 4**  
simulation with  
**DIANE**

Transparent to the user:

**same** Geant4 application code in **sequential** and **parallel** execution mode

*Results presented at CHEP06  
Publication in preparation*



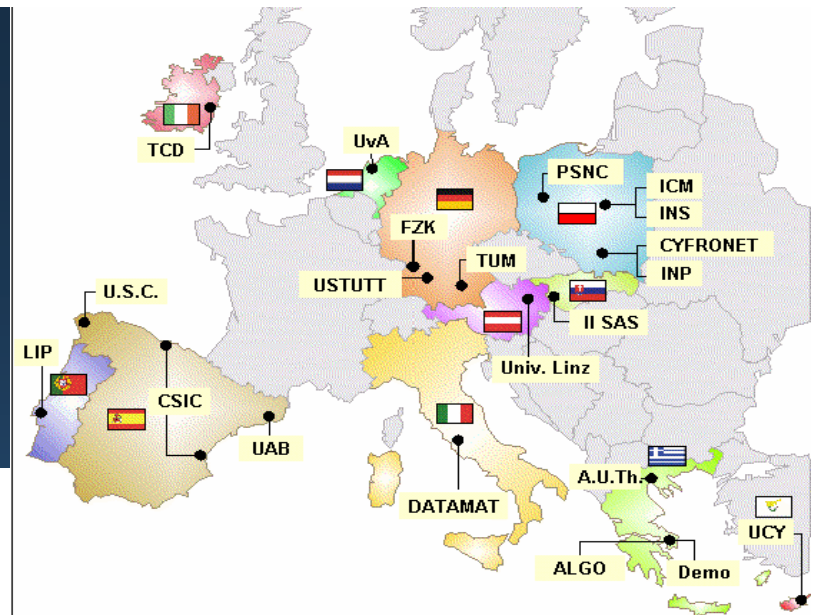
# Traceback from a run on grid testbed

Resource broker running in Portugal

Current #Grid setup (computing elements):

matchmaking CrossGrid computing elements

- aocegrid.uab.es:2119/jobmanager-pbs-workq
- bee001.ific.uv.es:2119/jobmanager-pbs-qgrid
- cgnode00.di.uoa.gr:2119/jobmanager-pbs-workq
- cms.fuw.edu.pl:2119/jobmanager-pbs-workq
- grid01.physics.auth.gr:2119/jobmanager-pbs-workq
- xg001.inp.demokritos.gr:2119/jobmanager-pbs-workq
- xgrid.icm.edu.pl:2119/jobmanager-pbs-workq
- zeus24.cyf-kr.edu.pl:2119/jobmanager-pbs-infinite
- zeus24.cyf-kr.edu.pl:2119/jobmanager-pbs-long
- zeus24.cyf-kr.edu.pl:2119/jobmanager-pbs-medium
- zeus24.cyf-kr.edu.pl:2119/jobmanager-pbs-short
- ce01.lip.pt:2119/jobmanager-pbs-qgrid



Spain

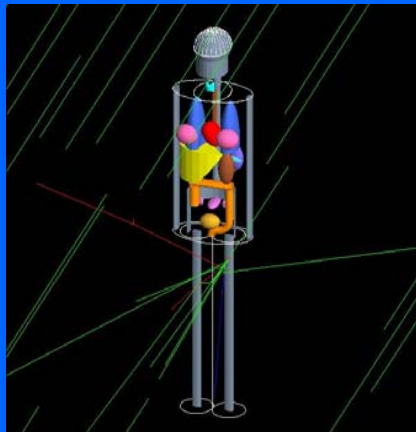
Greece

Poland

Portugal

# Scenario for Mars (and earth...)

Geant4 simulation treatment source + geometry from CT image or anthropomorphic phantom



Dose in organs at risk

Phase space input to nano-simulation

Geant4 simulation with biological processes at cellular level (cell survival, cell damage...)

Oncological risk to astronauts/patients  
Risk of nervous system damage

Geant4 simulation with physics at eV scale + DNA processes

# Geant 4

Powerful **geometry** and **physics** modelling  
in an advanced computing environment

*Wide spectrum of complementary and  
alternative physics models*

Multi-disciplinary  
dosimetry simulation

Precision of physics  
Versatility of experimental modelling

## Geant 4 DNA

Extensions for bio-molecular  
systems  
Physics processes at the eV scale  
**Biological** models

Multiple levels  
in the same simulation  
environment

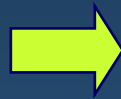
Conventional dosimetry  
Models at **cellular** level  
Models at **DNA** level

Rigorous software engineering  
Advanced object oriented technology  
in support of **physics versatility**

# Post-conclusions

What is the impact of what we are doing?

Software



Knowledge made **usable**



Feedback  
Improvement  
Extension

**Proposal**

Joint Geant4-DNA / COST Workshop

Common concrete **objectives**  
Collaborative projects



- Experimental measurements
- Theoretical models
- Software

*For those who may be interested: we organize **Geant4 Training Courses***