Geant 4

Simulation capabilities and application results

http://cern.ch/geant4/

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

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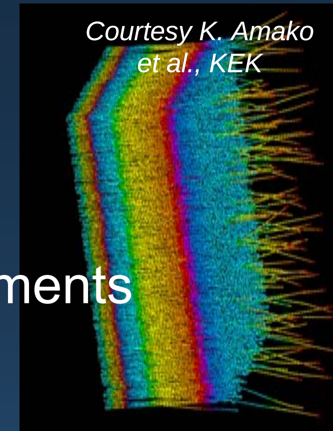
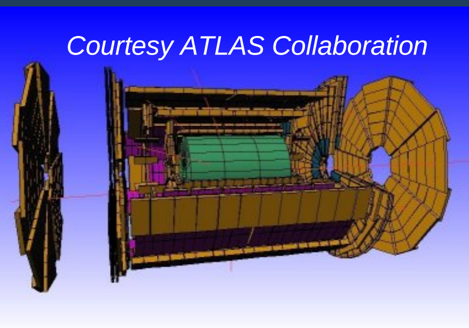
Geant 4

Courtesy CMS Collaboration



Courtesy K. Amako et al., KEK

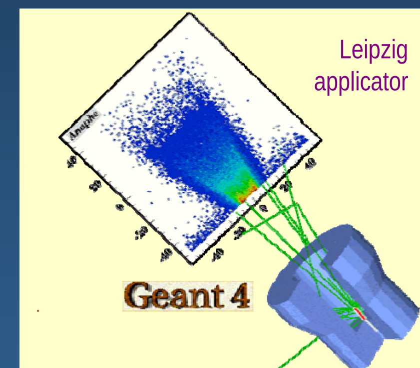
Born from the requirements of large scale HEP experiments

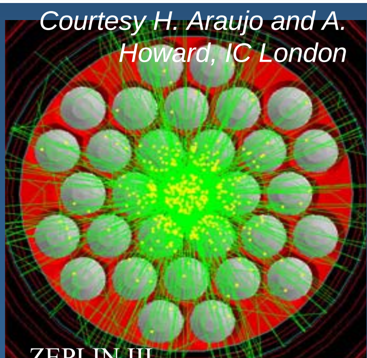


Courtesy ATLAS Collaboration

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…

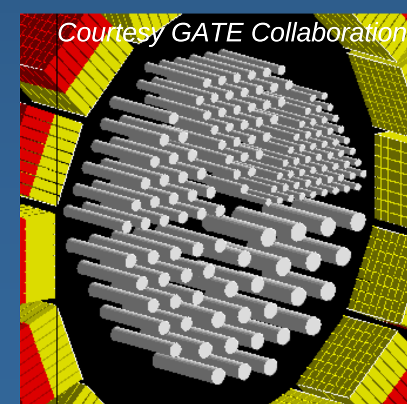




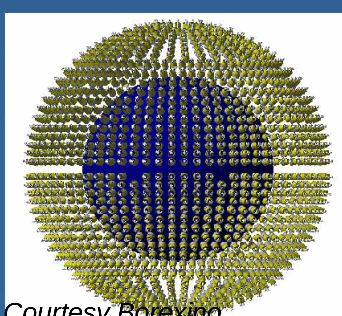
Courtesy H. Araujo and A. Howard, IC London

Courtesy R. Nartallo et al.,ESA

Most cited "engineering" publication in the past 2 years!



Courtesy GATE Collaboration



Courtesy Borexino

Technology transfer

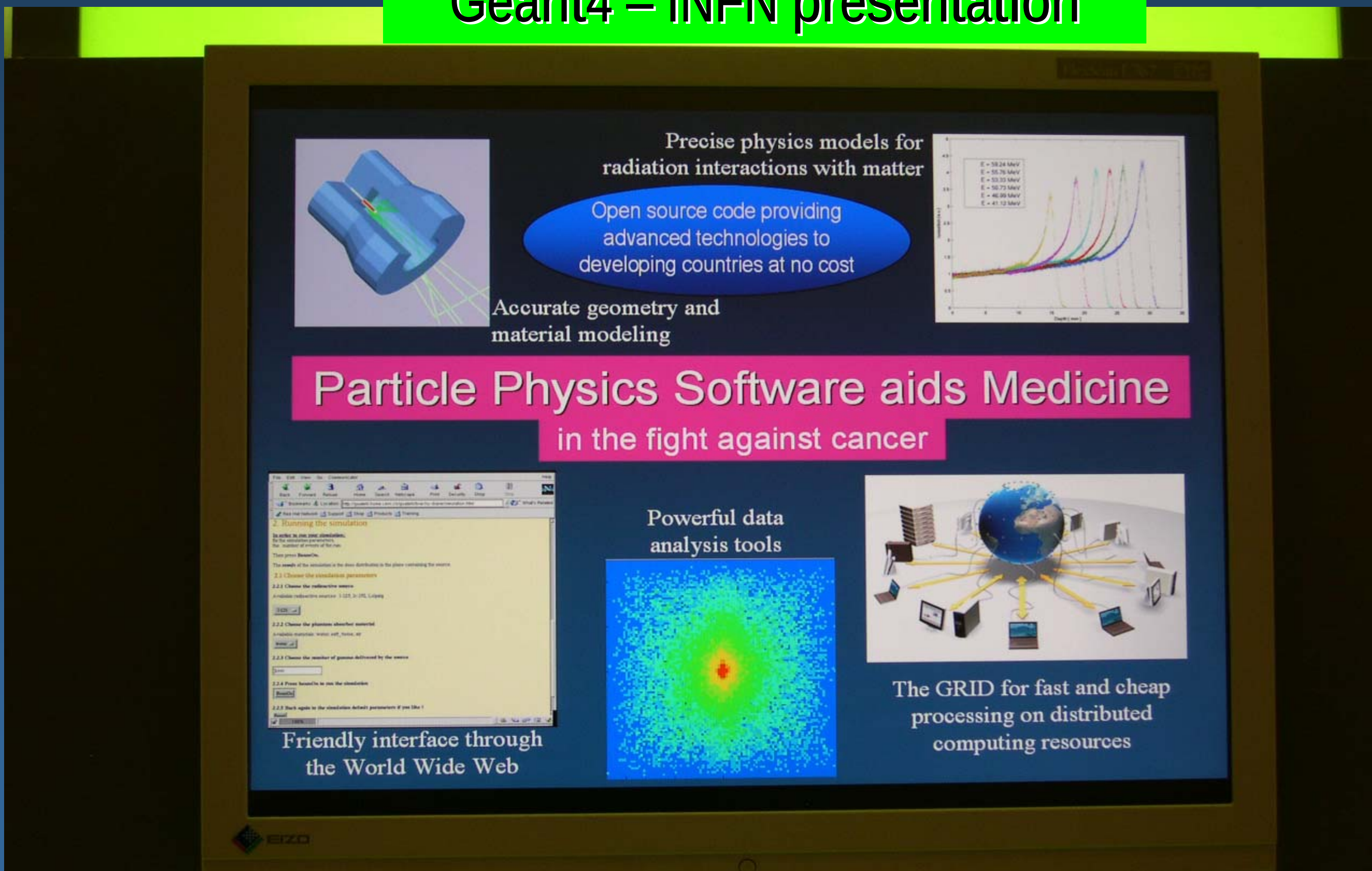
Particle physics software aids space and medicine

Geant4 is a showcase example of technology transfer from particle physics to other fields such as space and medical science […].

CERN Courier, June 2002

United Nations
World Summit on Information Society
Geneva, December 2003

Geant4 – INFN presentation

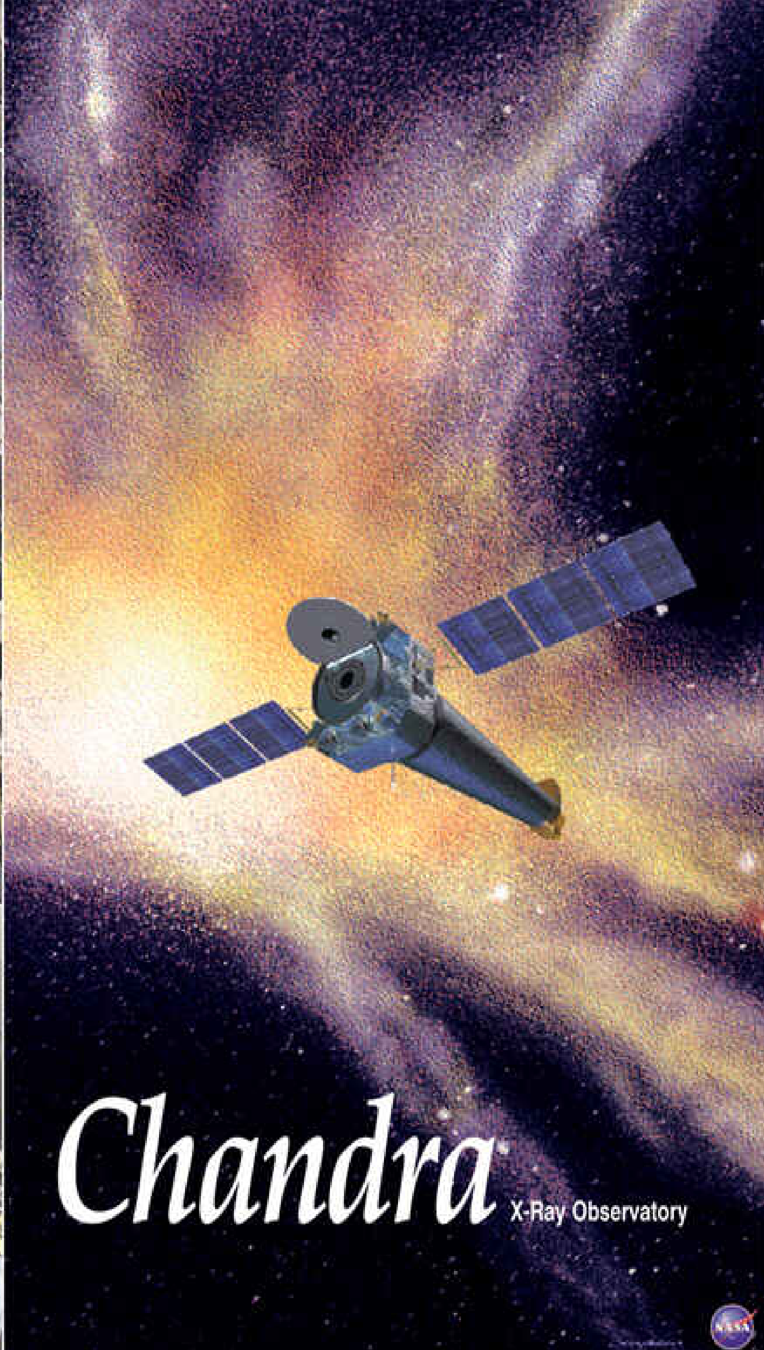


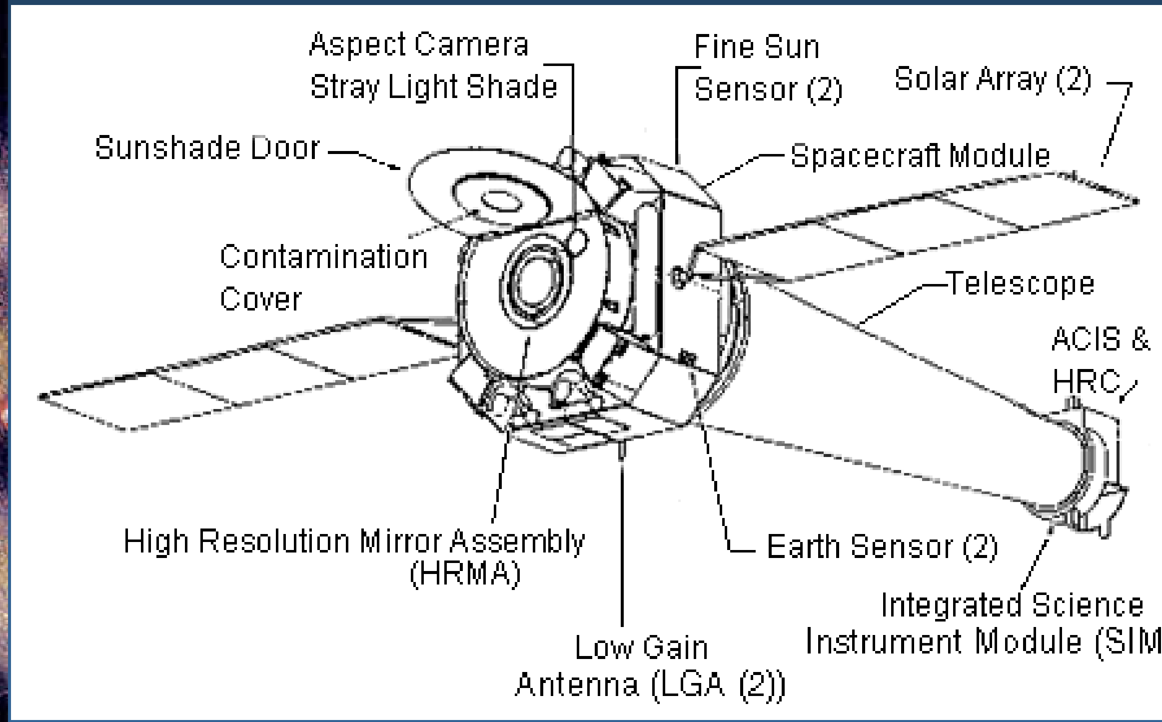
scientific…

Globalisation

Sharing requirements and functionality across diverse fields

Once upon a time there was a X-ray telescope...

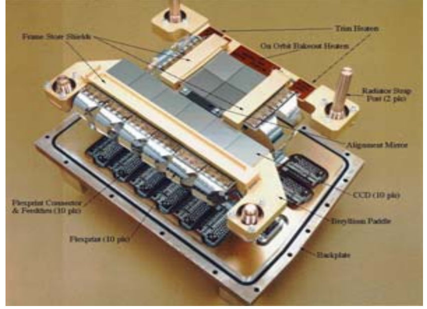




Courtesy of NASA/CXC/SAO

Chandra X-ray Observatory
Status Update

September 14, 1999
MSFC/CXC



CHANDRA CONTINUES TO TAKE SHARPEST IMAGES EVER; TEAM STUDIES INSTRUMENT DETECTOR CONCERN

Normally every complex space facility encounters a few problems during its checkout period; even though Chandra's has gone very smoothly, the science and engineering team is working a concern with a portion of one science instrument.

The team is investigating a **reduction in the energy resolution** of one of two sets of X-ray detectors in the Advanced Charge-coupled Device Imaging Spectrometer (ACIS) science instrument.

A series of diagnostic activities to characterize the degradation, identify possible causes, and test potential remedial procedures is underway.

The degradation appeared in the **front-side** illuminated Charge-Coupled Device (CCD) chips of the ACIS. The instrument's **back-side** illuminated chips have shown no reduction in capability and continue to perform flawlessly.

What could be the source of detector damage?

- Radiation belt electrons?
- Scattered in the mirror shells?
- Effectiveness of magnetic "brooms"?
- Electron damage mechanism? - NIEL?
- Other particles? Protons, cosmics?

Requirements for low energy p in Geant 4

GEANT4 LOW ENERGY ELECTROMAGNETIC PHYSICS

User Requirements Document

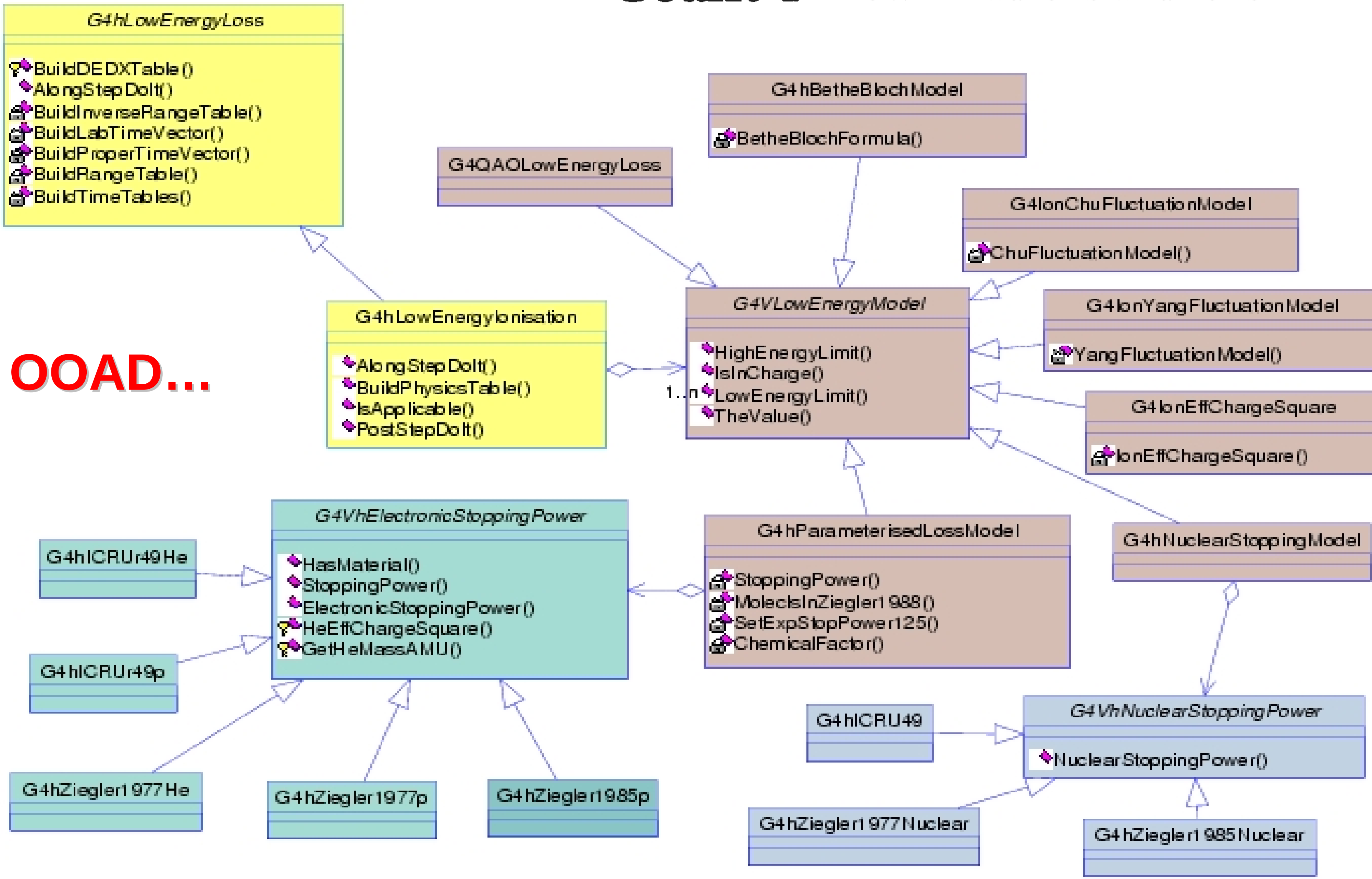
Status: in CVS repository

Version: 2.4
Project: Geant4-LowE
Reference: LowE-URD-V2.4
Created: 22 June 1999
Last modified: 26 March 2001
Prepared by: Petteri Nieminen (ESA) and Maria Grazia Pia (INFN)

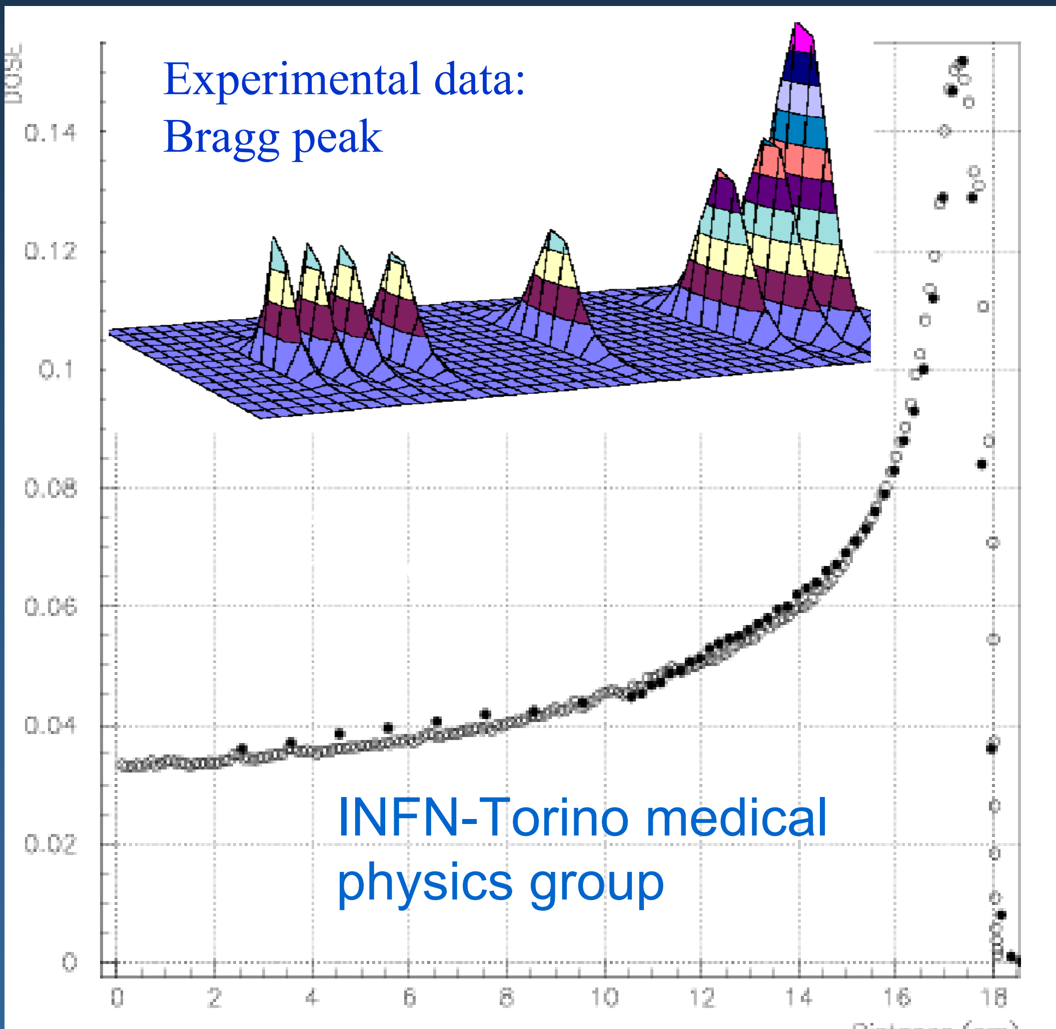
- **UR 2.1** The user shall be able to simulate electromagnetic interactions of positive charged hadrons down to < 1 KeV.
- **Need**: *Essential*
- **Priority**: *Required by end 1999*
- **Stability**: *Stable*
- **Source**: *Medical physics groups, PIXE*
- **Clarity**: *Clear*
- **Verifiability**: *Verified*

Geant 4 LowE Hadrons and Ions

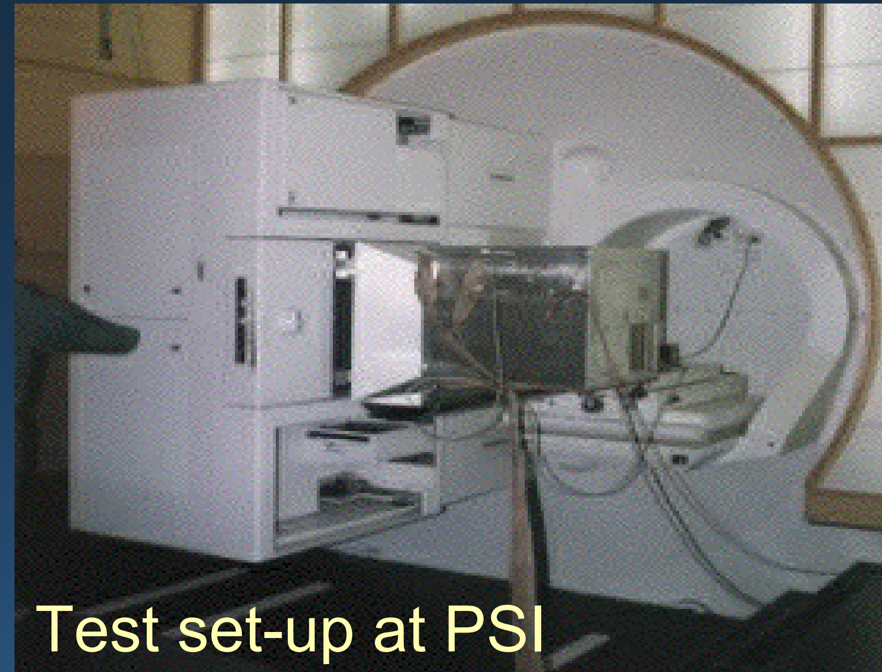
OOAD...

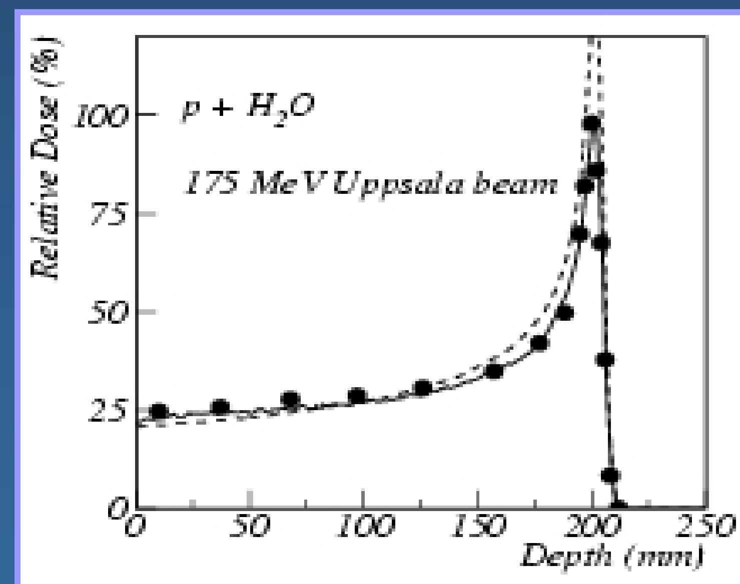


…and validation



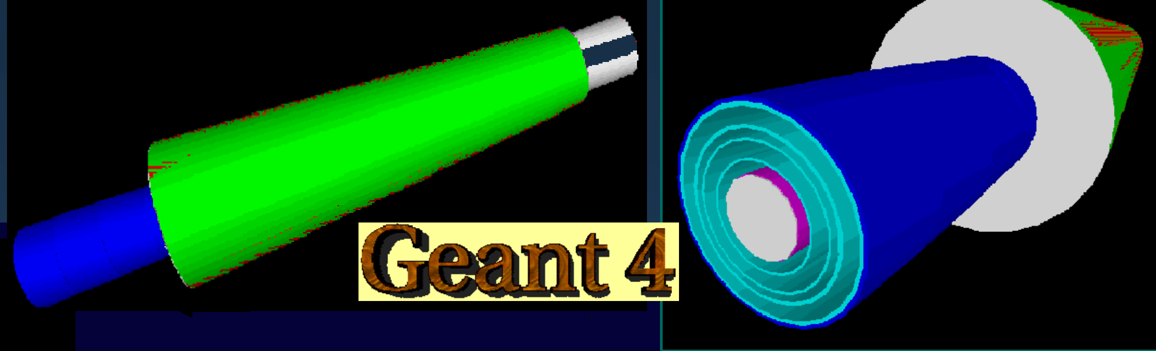
Courtesy of R. Gotta, Thesis

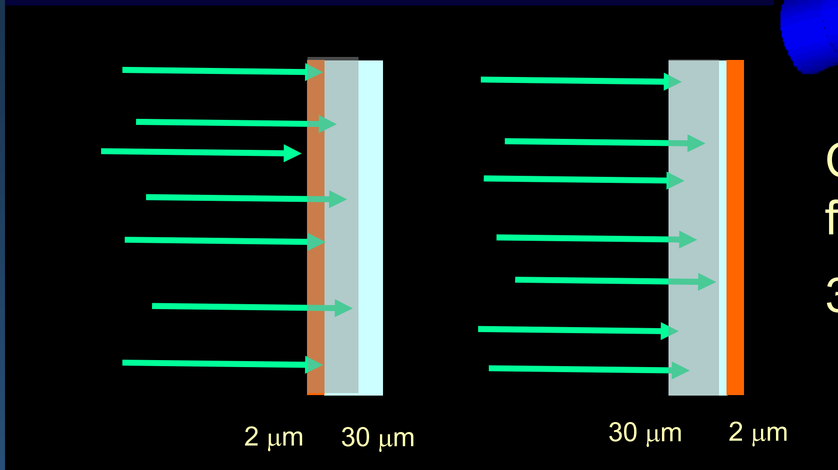




Geant4 LowE Working Group

ESA Space Environment & Effects Analysis Section

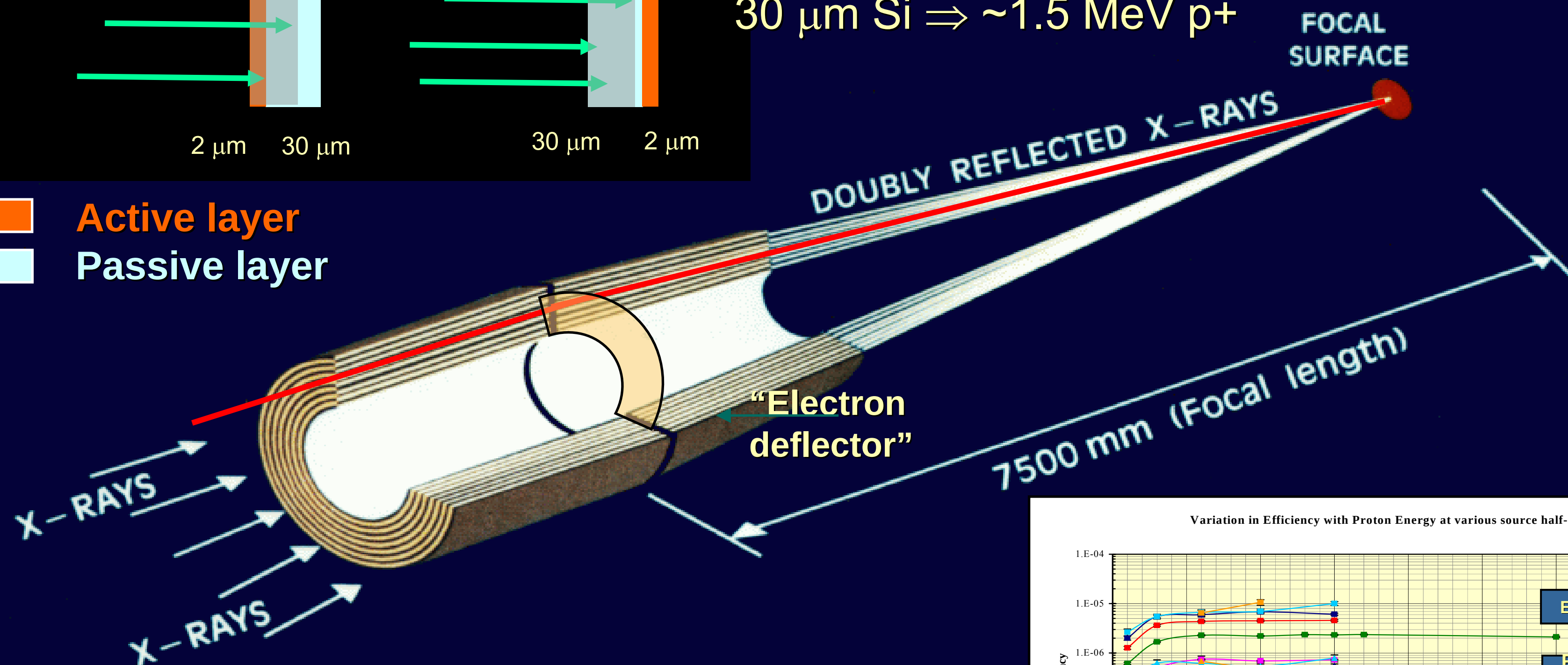


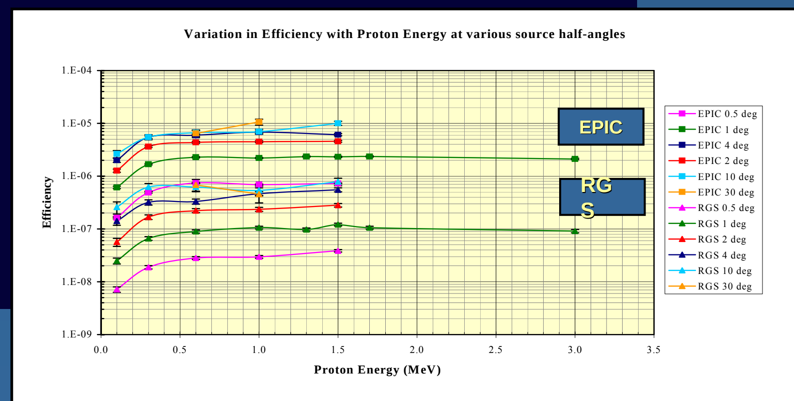


- **Active layer**
- **Passive layer**

CCD displacement damage: front vs. back-illuminated

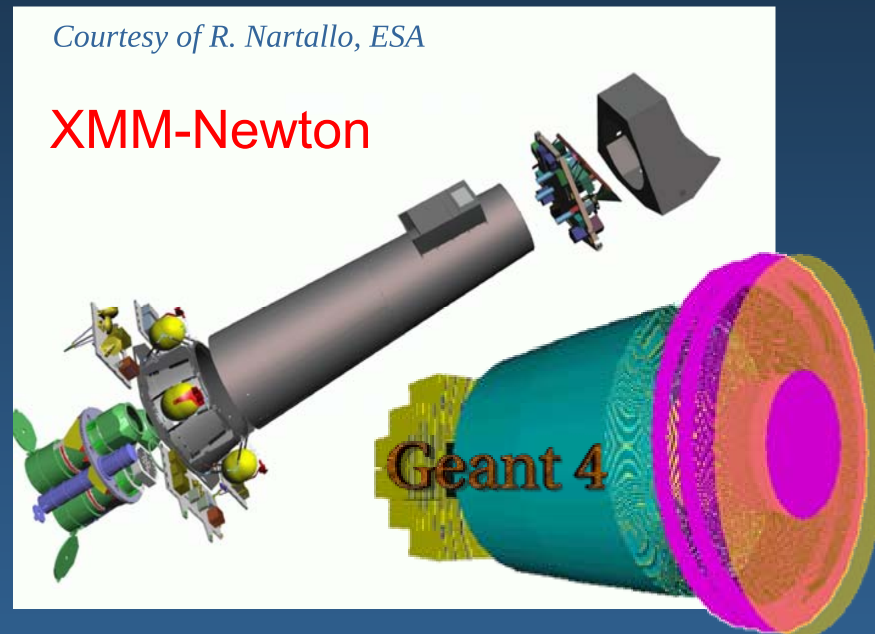
30 μm Si ⇒ ~1.5 MeV p+

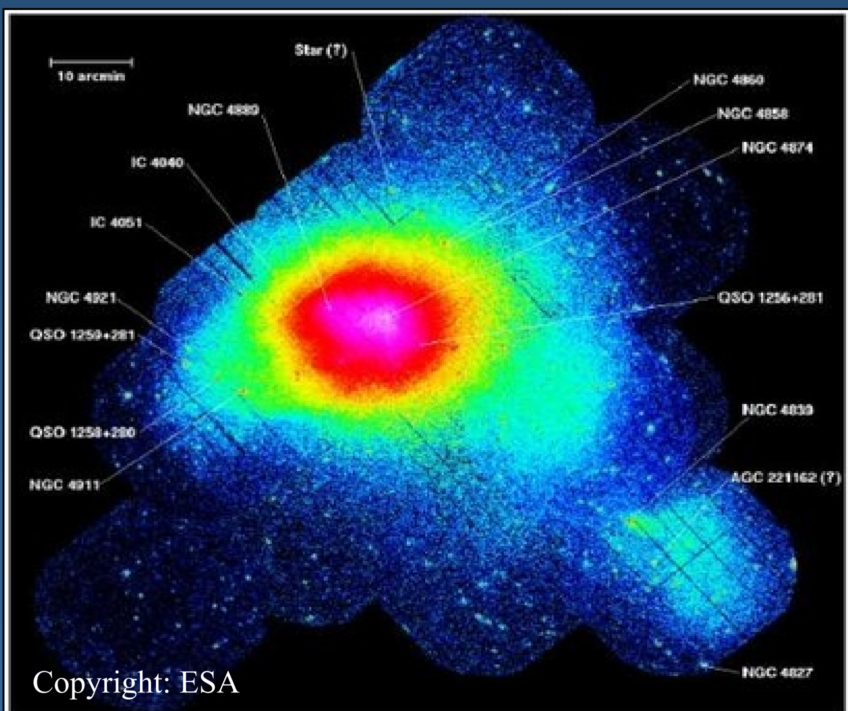




Low-E (~100 keV to few MeV), low-angle (~0°-5°) proton scattering

XMM-Newton was launched on 10 December 1999





Simulation can be mission-critical!

(not only in a space mission…)

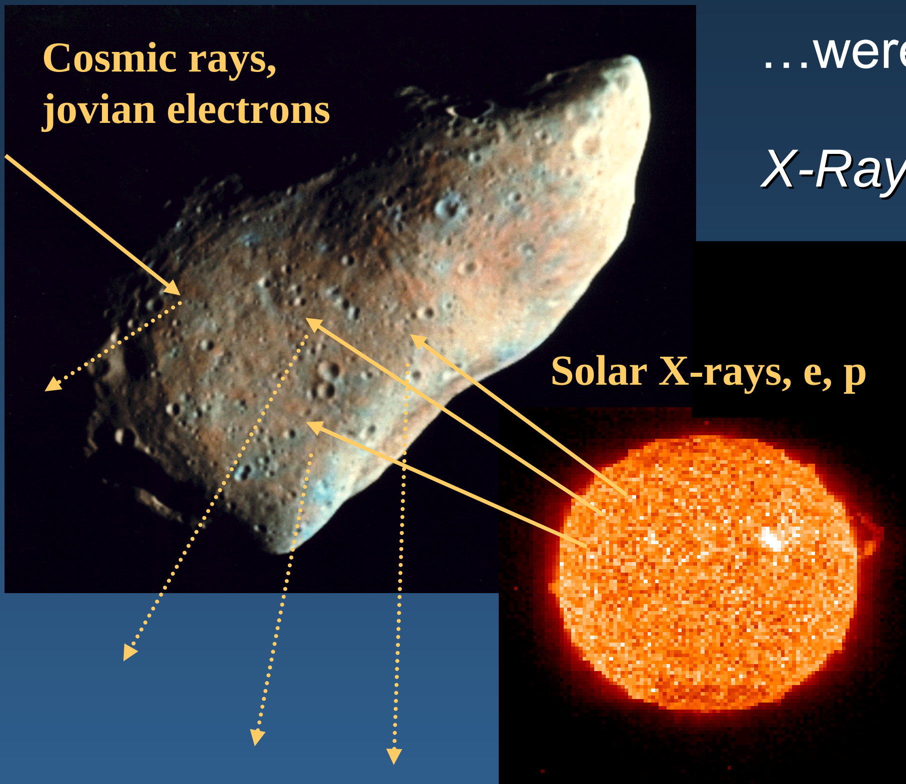
EPIC-PN image of the Coma Cluster

…and the other way round

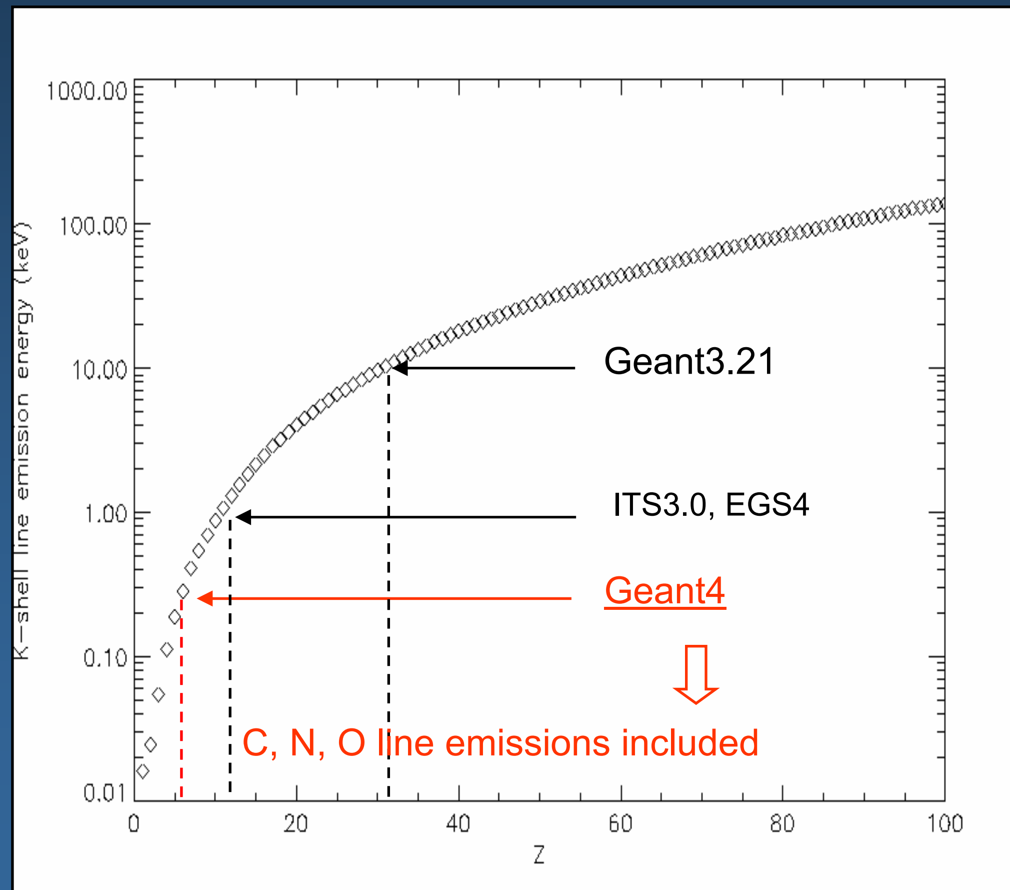
Geant4 low energy e, γ extensions

…were triggered by astrophysics requirements

X-Ray Surveys of Planets, Asteroids and Moons



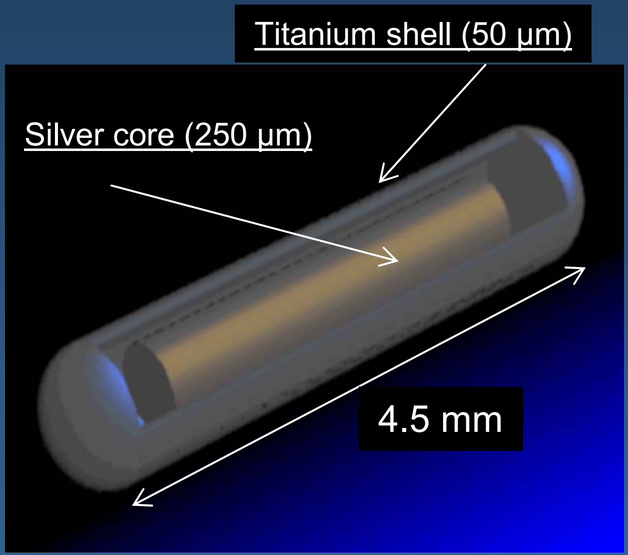
Courtesy SOHO EIT

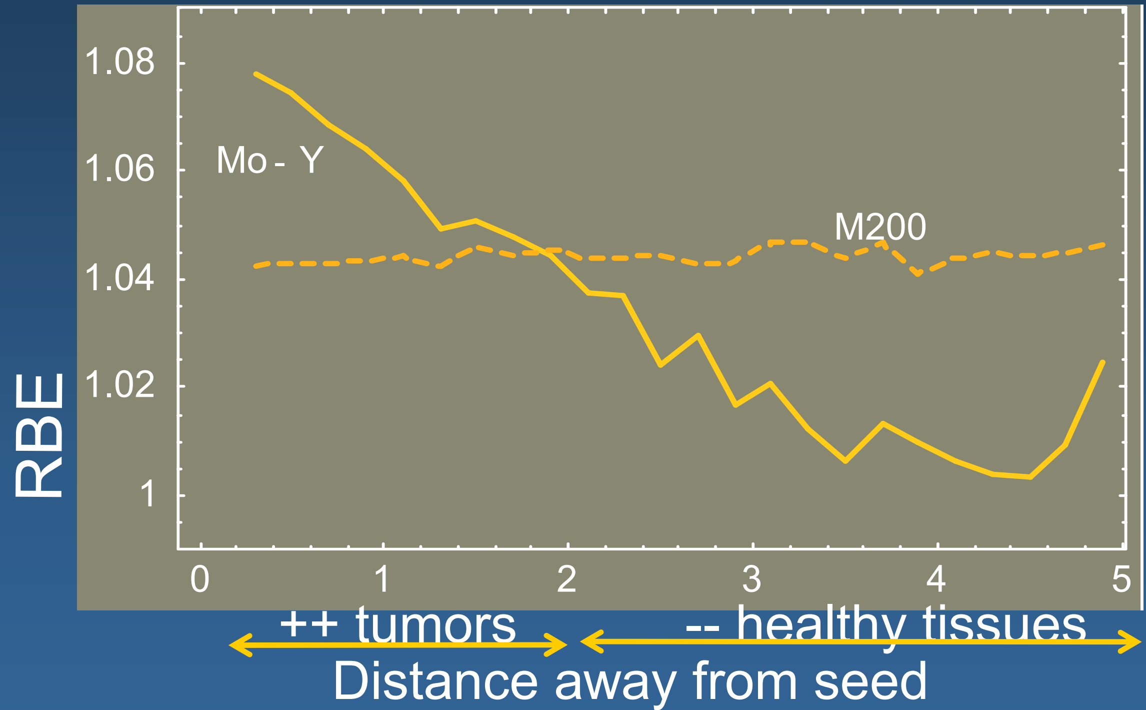


Induced X-ray line emission:
indicator of target composition
(~100 μm surface layer)

…the first user application

Goal: improve the biological effectiveness of titanium encapsulated ^{125}I sources in permanent prostate implants by exploiting X-ray fluorescence



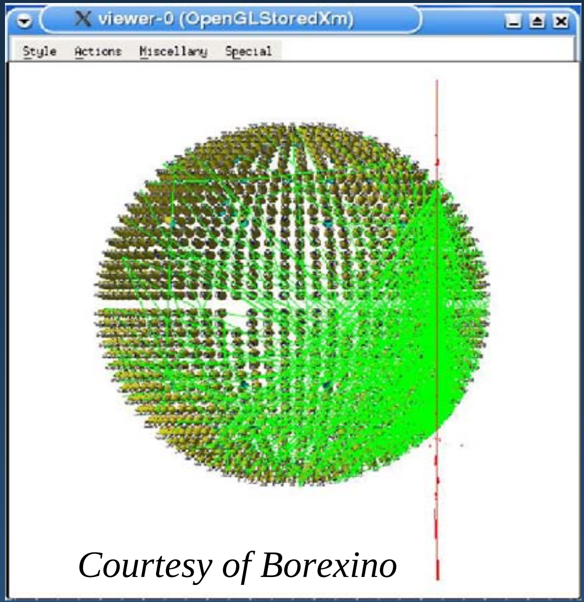


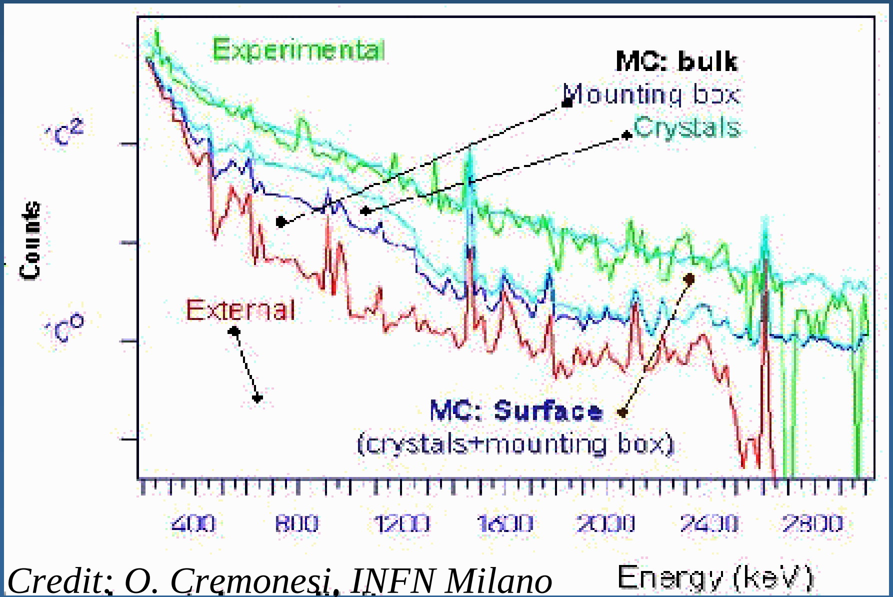
R. Taschereau, R. Roy, J. Pouliot

Centre Hospitalier Universitaire de Quebec, Dept. de radio-oncologie, Canada

Univ. Laval, Dept. de Physique, Canada

Univ. of California, San Francisco, Dept. of Radiation Oncology, USA





...back to HEP

- Similar requirements on low energy physics from underground neutrino and dark matter experiments
- Recent interest on these physics models from LHC for precision detector simulation

Publications on Medical Physics in 2004-2005 (1)

1) Monte Carlo derivation of TG-43 dosimetric parameters for radiation therapy resources and 3M Cs-137 sources ,
J. Pérez-Calatayud, D. Granero, F. Ballester, E. Casal, R. Cases, and S. Agramunt, Med. Phys. **32**, 2464 (2005)

2) Octree based compression method of DICOM images for voxel number reduction and faster Monte Carlo
V Hubert-Tremblay, L Archambault, L Beaulieu, and R Roy, Med. Phys. **32**, 2413 (2005)

3) Simulation of Dosimetric Properties of Very-High Energy Laser-Accelerated Electron Beams
T Fuchs, H Szymanowski, Y Glinec, J Faure, V Malka, and U Oelfke, Med. Phys. **32**, 2163 (2005)

4) Quantum Efficiency of An MCP Detector: Monte Carlo Calculation,
PM Shikhaliev, JL Ducote, T Xu, and S Molloi, Med. Phys. **32**, 2158 (2005)

6) The Use of a Miniature Multileaf Collimator in Stereotactic Proton Therapy
R Slopsema, H Paganetti, H Kooy, M Bussiere, J Sisterson, J Flanz, and T Bortfeld, Med. Phys. **32**, 2088 (2005)

7) Simulation of Organ Specific Secondary Neutron Dose in Proton Beam Treatments
H Jiang, B Wang, X Xu, H Suit, and H Paganetti, Med. Phys. **32**, 2071 (2005)

8) Study of Truncated Cone Filters Using GEANT4
T Himukai, Y Takada, and R Kohno, Med. Phys. **32**, 2030 (2005)

9) Proton Dose Calculation Using Monte-Carlo-Validated Pencil Beam Database for KonRad Treatment Planning System
A Trofimov, A Knopf, H Jiang, T Bortfeld, and H Paganetti, Med. Phys. **32**, 2030 (2005)

10) Monte-Carlo Investigation of Proton-Generated Radioactivity in a Multileaf Collimator for a Proton Therapy Facility
J McDonough, D Goulart, M Baldytchev, P Bloch, and R Maughan, Med. Phys. **32**, 2030 (2005)

11) Energy Distributions of Proton Interactions in MCNPX and GEANT4 Codes Using a Slab Target
B Wang, X George Xu, H Jiang, and H Paganetti, Med. Phys. **32**, 2029 (2005)

12) Monte Carlo Calculation of the TG-43 Dosimetric Parameters of a New BEBIG Ir-192 HDR Source
F Ballester, E Casal, D Granero, J Perez-Calatayud, S Agramunt, and R Cases, Med. Phys. **32**, 1952 (2005)

Publications on Medical Physics in 2004-2005 (2)

13) Comparison of Pencil Beam Algorithm and Monte Carlo Dose Calculation for Proton Therapy of Paranasal Sinus Cancer
H Jiang, J Adams, S Rosenthal, S Kollipara, and H Paganetti, Med. Phys. **32**, 2028 (2005)

14) Clinical Implementation of Proton Monte Carlo Dose Calculation
H Paganetti, H Jiang, and S Kollipara, Med. Phys. **32**, 2028 (2005)

15) Validation of a Monte Carlo Algorithm for Simulation of Dispersion Due to Scattering of a Monoenergetic Proton Beam
D Goulart, S Avery, R Maughan, and J McDonough, Med. Phys. **32**, 2019 (2005)

16) Monte Carlo Simulations of the Dosimetric Characteristics of a New Multileaf Collimator
M Tacke, H Szymanowski, C Schulze, S Nuss, E Wehrwein, S Leidenberger, and U Oelfke, Med. Phys. **32**, 2018 (2005)

17) Verification of Monte Carlo Simulations of Proton Dose Distributions in Biological Media
H Szymanowski, S Nill, and U Oelfke, Med. Phys. **32**, 2014 (2005)

18) Octree Based Compression Method of DICOM Images for Voxel Number Reduction and Faster Monte Carlo Simulations
V Hubert-Tremblay, L Archambault, L Beaulieu, and R Roy, Med. Phys. **32**, 2013 (2005)

19) Design Characteristics of a MLC for Proton Therapy
S Avery, D Goulart, R Maughan, and J McDonough, Med. Phys. **32**, 2012 (2005)

20) Clinical Impact of Seed Density and Prostate Elemental Composition On Permanent Seed Implant Dosimetry
J Carrier, F Therriault-Proulx, R Roy, and L Beaulieu, Med. Phys. **32**, 2011 (2005)

21) Monte Carlo Dosimetric Study of the New BEBIG Co-60 HDR Source
J Perez-Calatayud, D Granero, F Ballester, E Casal, S Agramunt, and R Cases, Med. Phys. **32**, 1958 (2005)

22) Monte Carlo Derivation of TG-43 Dosimetric Parameters for Radiation Therapy Resources and 3M Cs-137 Sources
E Casal, D Granero, F Ballester, J Perez-Calatayud, S Agramunt, and R Cases, Med. Phys. **32**, 1952 (2005)

Publications on Medical Physics in 2004-2005 (3)

23) PSF and S/P in Mammography: A Validation of Simulations Using the GEANT4 Code
V Grabski, M-E Brandan, C. Ruiz-Trejo, and Y. Villaseñor, Med. Phys. **32**, 1911 (2005)

24) Validation of GATE Monte Carlo Simulations of the Noise Equivalent Count Rate and Image Quailty for the GE Discovery LS PET Scanner
CR Schmidtlein, AS Kirov, SA Nehmeh, LM Bidaut, YE Erdi, KA Hamacher, JL Humm, and HI Amols, Med. Phys. **32**, 1900 (2005)

25) SU-EE-A2-05: Accuracy in the Determination of Microcalcification Thickness in Digital Mammography
M-E Brandan and V Grabski, Med. Phys. **32**, 1898 (2005)

26) Accuracy of the photon and electron physics in GEANT4 for radiotherapy applications
Emily Poon and Frank Verhaegen , Med. Phys. **32**, 1696 (2005)

27) Density resolution of proton computed tomography,
Reinhard W. Schulte, Vladimir Bashkirov, Márgio C. Loss Klock, Tianfang Li, Andrew J. Wroe, Ivan Evseev, David C. Williams, and Todd Satogata, Med. Phys. **32**, 1035 (2005)

28) The role of nonelastic reactions in absorbed dose distributions from therapeutic proton beams in different medium
Andrew J. Wroe, Iwan M. Cornelius, and Anatoly B. Rosenfeld, Med. Phys. **32**, 37 (2005)

29) Monte Carlo and experimental derivation of TG43 dosimetric parameters for CSM-type Cs-137 sources
J. Pérez-Calatayud, D. Granero, E. Casal, F. Ballester, and V. Puchades, Med. Phys. **32**, 28 (2005)

30) Dosimetric study of the 15 mm ROPES eye plaque
D. Granero, J. Pérez-Calatayud, F. Ballester, E. Casal, and J. M. de Frutos, Med. Phys. **31**, 3330 (2004)

31) Monte Carlo dosimetric study of Best Industries and Alpha Omega Ir-192 brachytherapy seeds
F. Ballester, D. Granero, J. Pérez-Calatayud, E. Casal, and V. Puchades, Med. Phys. **31**, 3298 (2004)

Publications on Medical Physics in 2004-2005 (4)

32) Adaptation of GEANT4 to Monte Carlo dose calculations based on CT data
H. Jiang and H. Paganetti, Med. Phys. **31**, 2811 (2004)

33) Accurate Monte Carlo simulations for nozzle design, commissioning and quality assurance for a proton radiation therapy facility
H. Paganetti, H. Jiang, S.-Y. Lee, and H. M. Kooy, Med. Phys. **31**, 2107 (2004)

34) Phantom size in brachytherapy source dosimetric studies
J. Pérez-Calatayud, D. Granero, and F. Ballester, Med. Phys. **31**, 2075 (2004)

35) Monte Carlo dosimetric characterization of the Cs-137 selectron/LDR source: Evaluation of applicator attenuation and superposition approximation effects
J. Pérez-Calatayud, D. Granero, F. Ballester, V. Puchades, and E. Casal, Med. Phys. **31**, 493 (2004)

36) Validation of GEANT4, an object-oriented Monte Carlo toolkit, for simulations in medical physics
J.-F. Carrier, L. Archambault, L. Beaulieu, and R. Roy, Med. Phys. **31**, 484 (2004)

37) Dosimetry characterization of 32P intravascular brachytherapy source wires using Monte Carlo codes PENELOPE and GEANT4,
Javier Torres, Manuel J. Buades, Julio F. Almansa, Rafael Guerrero, and Antonio M. Lallena, Med. Phys. **31**, 296 (2004)

Publications on Physics in Medicine and Biology in 2004-2005 (1)

1) Neutrons from fragmentation of light nuclei in tissue-like media: a study with the GEANT4 toolkit
Pshenichnov I, Mishustin I, Greiner W, Phys Med Biol. **50** No 23, 5493-5507.

2) Monte Carlo dosimetric study of the BEBIG Co-60 HDR source.
Ballester F, Granero D, Perez-Calatayud J, Casal E, Agramunt S, Cases R., Phys Med Biol. **50** No 21, 309-316

3) Monte Carlo simulation and scatter correction of the GE advance PET scanner with SimSET and Geant4
Barret O, Carpenter TA, Clark JC, Ansorge RE, Fryer TD, Phys Med Biol. **50** No 20, 4823-4840.

4) GATE: a simulation toolkit for PET and SPECT
S Jan, G Santin, D Strul, S Staelens, K Assié, D Autret, S Avner, R Barbier, M Bardiès, P M Bloomfield, D Brasse, V Breton, P Bruyndonckx, I Buvat, A F Chatziioannou, Y Choi, Y H Chung, C Comtat, D Donnarieix, L Ferrer, S J Glick, C J Groiselle, Guez, P-F Honore, S Kerhoas-Cavata, A S Kirov, V Kohli, M Koole, M Krieguer, D J van der Laan, F Lamare, G Largeron, Lartizien, D Lazaro, M C Maas, L Maigne, F Mayet, F Melot, C Merheb, E Pennacchio, J Perez, U Pietrzyk, F R Rannou, Rey, D R Schaart, C R Schmidtlein, L Simon, T Y Song, J-M Vieira, D Visvikis, R Van de Walle, E Wieërs and C Morel
Phys. Med. Biol. **49** No 19, 4543-4561

5) Monte Carlo simulations of a scintillation camera using GATE: validation and application modelling
S Staelens, D Strul, G Santin, S Vandenberghe, M Koole, Y D'Asseler, I Lemahieu and R V de Walle
Phys. Med. Biol. **48** No 18, 3021-3042

6) Simulation of organ-specific patient effective dose due to secondary neutrons in proton radiation treatment
Hongyu Jiang, Brian Wang, X George Xu, Herman D Suit and Harald Paganetti
Phys. Med. Biol. **50** No 18, 4337-4353

7) Validation of the Monte Carlo simulator GATE for indium-111 imaging
K Assié, I Gardin, P Véra and I Buvat, *Phys. Med. Biol.* **50** No 13, 3113-3125

Publications on Physics in Medicine and Biology in 2004-2005 (2)

8) Integrating a MRI scanner with a 6 MV radiotherapy accelerator: dose increase at tissue–air interfaces in a lateral magnetic field due to returning electrons
A J E Raaijmakers, B W Raaymakers and J J W Lagendijk, Phys. Med. Biol. **50** No 7, 1363-1376

9) Consistency test of the electron transport algorithm in the GEANT4 Monte Carlo code
Emily Poon, Jan Seuntjens and Frank Verhaegen, Phys. Med. Biol. **50** No 4, 681-694

10) Monte Carlo evaluation of kerma in an HDR brachytherapy bunker
J Pérez-Calatayud, D Granero, F Ballester, E Casal, V Crispin, V Puchades, A León and G Verdú,
Phys. Med. Biol. **49** No 24, 389-396

11) Optimizing Compton camera geometries
Sudhakar Chelikani, John Gore and George Zubal, Phys. Med. Biol. **49** No 8,1387-1408

12) Four-dimensional Monte Carlo simulation of time-dependent geometries
H Paganetti, Phys. Med. Biol. **49** No 6, 75-81

13) Validation of the GATE Monte Carlo simulation platform for modelling a CsI(Tl) scintillation camera dedicated to small-animal imaging
D Lazaro, I Buvat, G Loudos, D Strul, G Santin, N Giokaris, D Donnarieix, L Maigne, V Spanoudaki, S Styliaris, S Staelens and V Breton, Phys. Med. Biol. **49** No 2, 271-285

14) Monte Carlo simulations of a scintillation camera using GATE: validation and application modelling
S Staelens, D Strul, G Santin, S Vandenberghe, M Koole, Y D'Asseler, I Lemahieu and R V de Walle
Phys. Med. Biol. **48** No 18, 3021-3042

…and many more: publications in IEEE Trans. Nucl. Sci. and IEEE Trans. Med. Imag. etc.

Creativity

Exotic Geant4 applications…

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

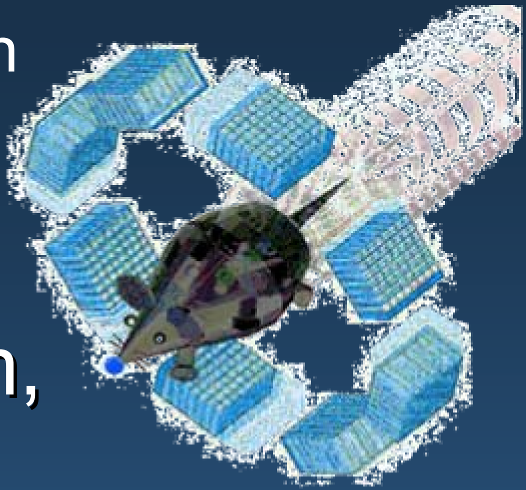
Integrating the Sterile Insect
and Related Nuclear and Other Techniques

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

Geant4 Application for Tomographic Emission



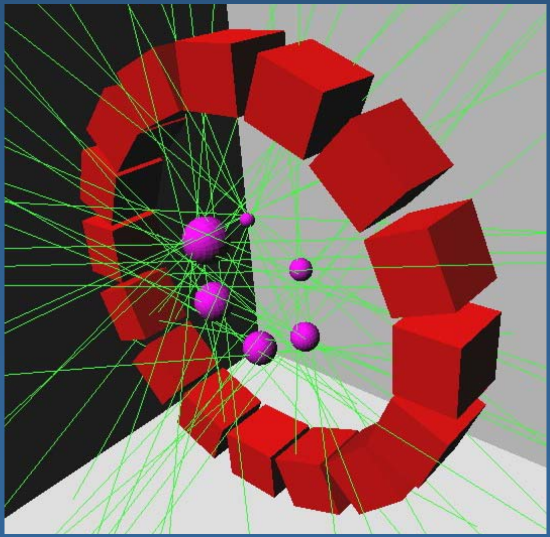
GATE

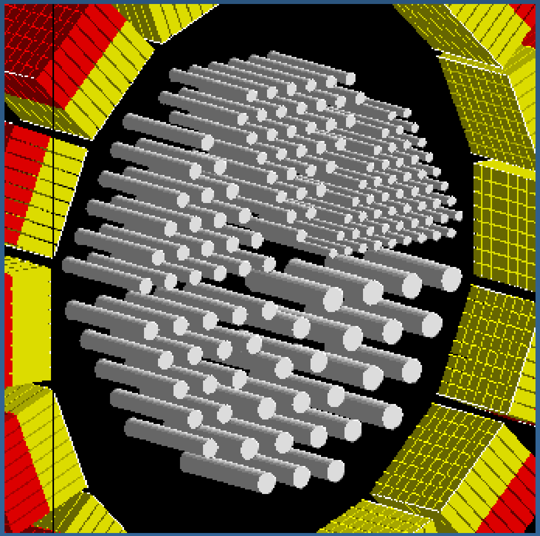
a Geant4 based simulation platform, designed for PET and SPECT

GATE Collaboration

Released as an open source software system under GPL

> 400 registered users worldwide





What is Geant 4?

OO Toolkit for the simulation of next generation HEP detectors

...of the current generation

...not only of HEP detectors

also…

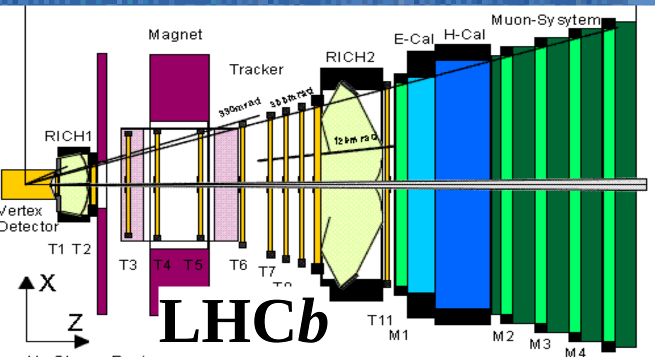
An experiment of distributed software production and management

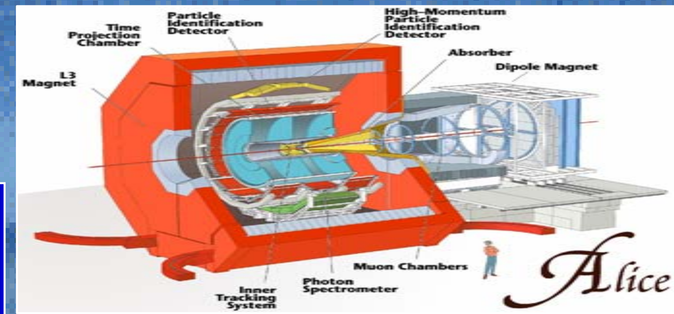
An experiment of application of rigorous software engineering methodologies and of the Object Oriented technology to the HEP environment

R&D phase: **RD44**, 1994 - 1998

1st release: December 1998

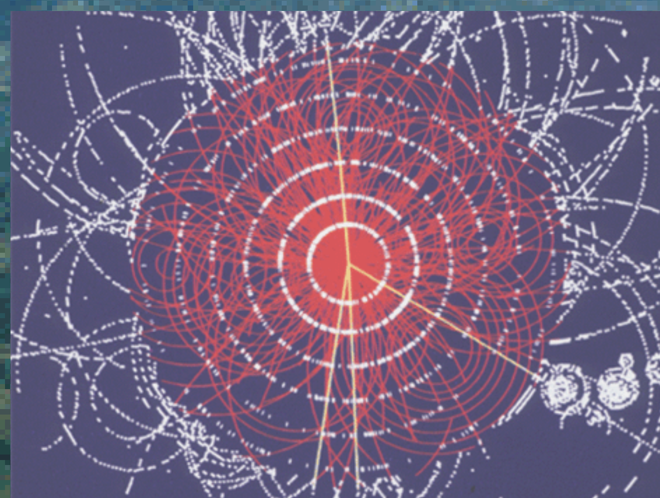
2 new releases/year since then

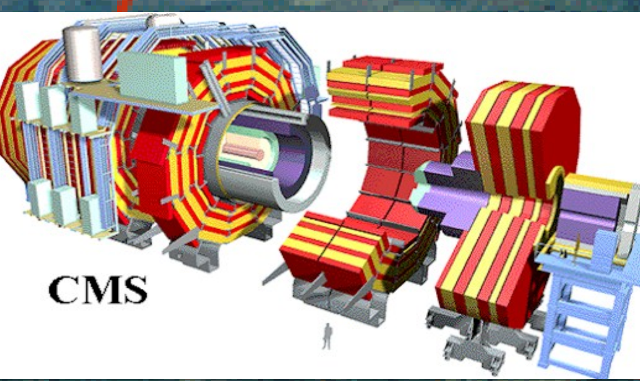


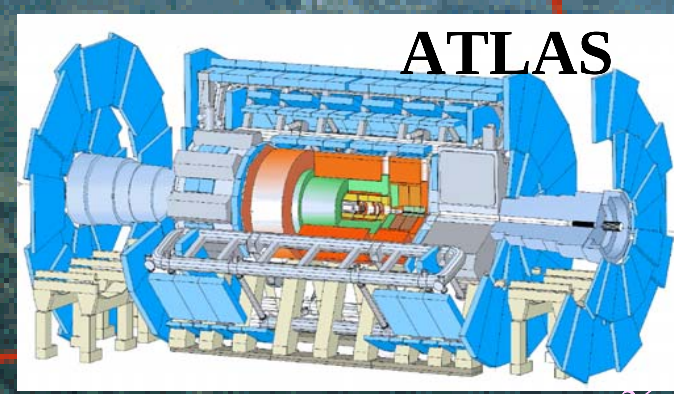


Complex physics
Complex detectors
20 years software life-span

LHC







From deep underground…

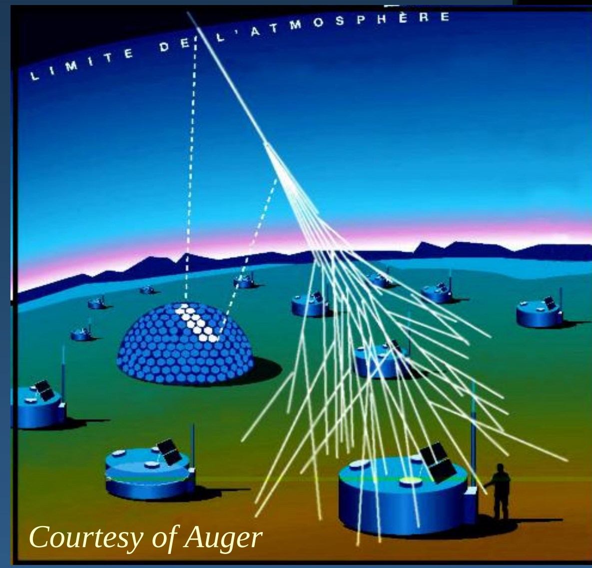
…to space

Courtesy of ESA

X and γ astronomy, gravitational waves, radiation damage to components etc.

Dark matter and ν experiments

Courtesy UKDM, Boulby Mine



Courtesy of Auger

Cosmic ray experiments

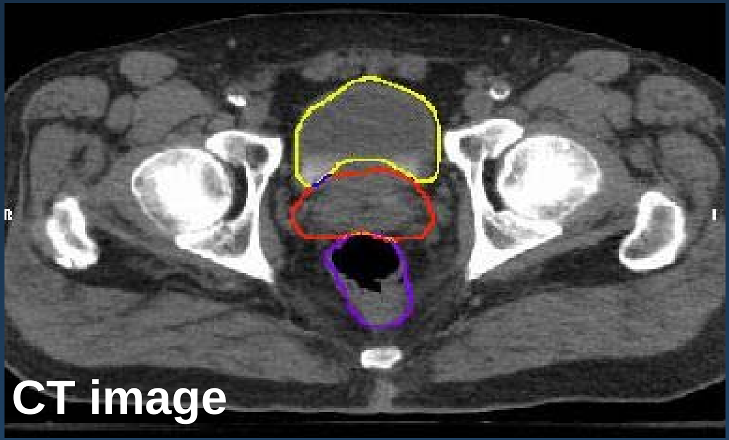
Variety of requirements from diverse applications

Physics from the eV to the PeV scale	Detectors, spacecrafts and environment

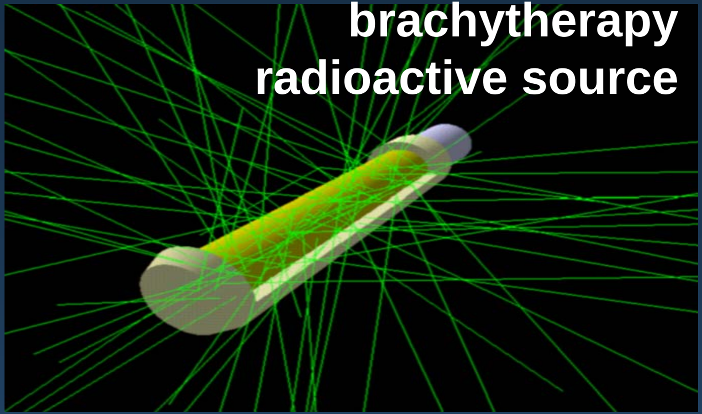
For such experiments software is often **mission critical**

Require reliability, rigorous software engineering standards

Maria Grazia Pia, *INFN Genova*



Medical Physics

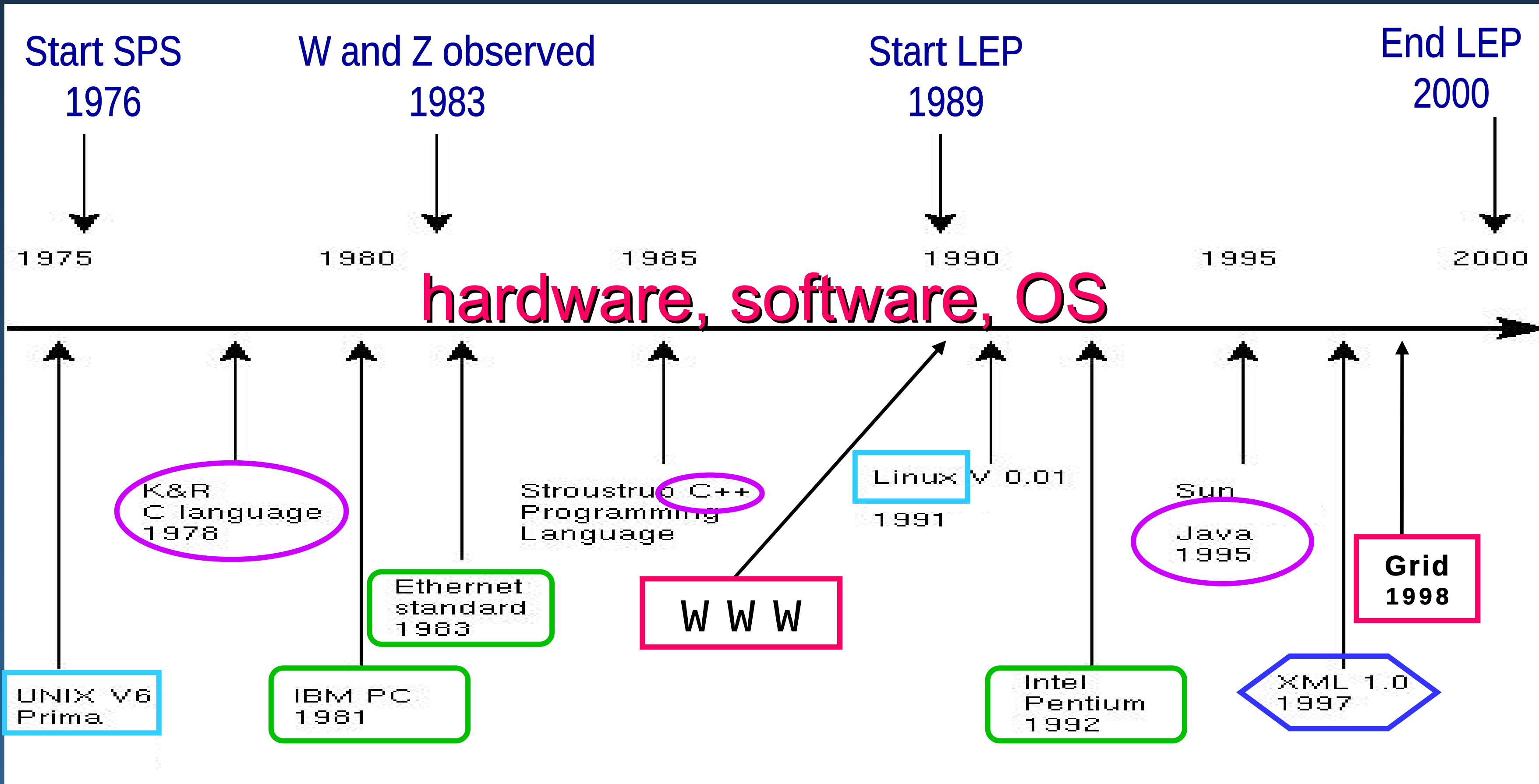


from hospitals…

…to Mars

- Accurate modelling of radiation sources, devices and human body
- Precision of physics
- Reliability
- Easy configuration and friendly interface
- Speed

…in a fast changing computing environment



…and don't forget changes of requirements!

Evolution towards greater diversity ⇒ we must **anticipate changes**

Strategic vision

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

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

The foundation

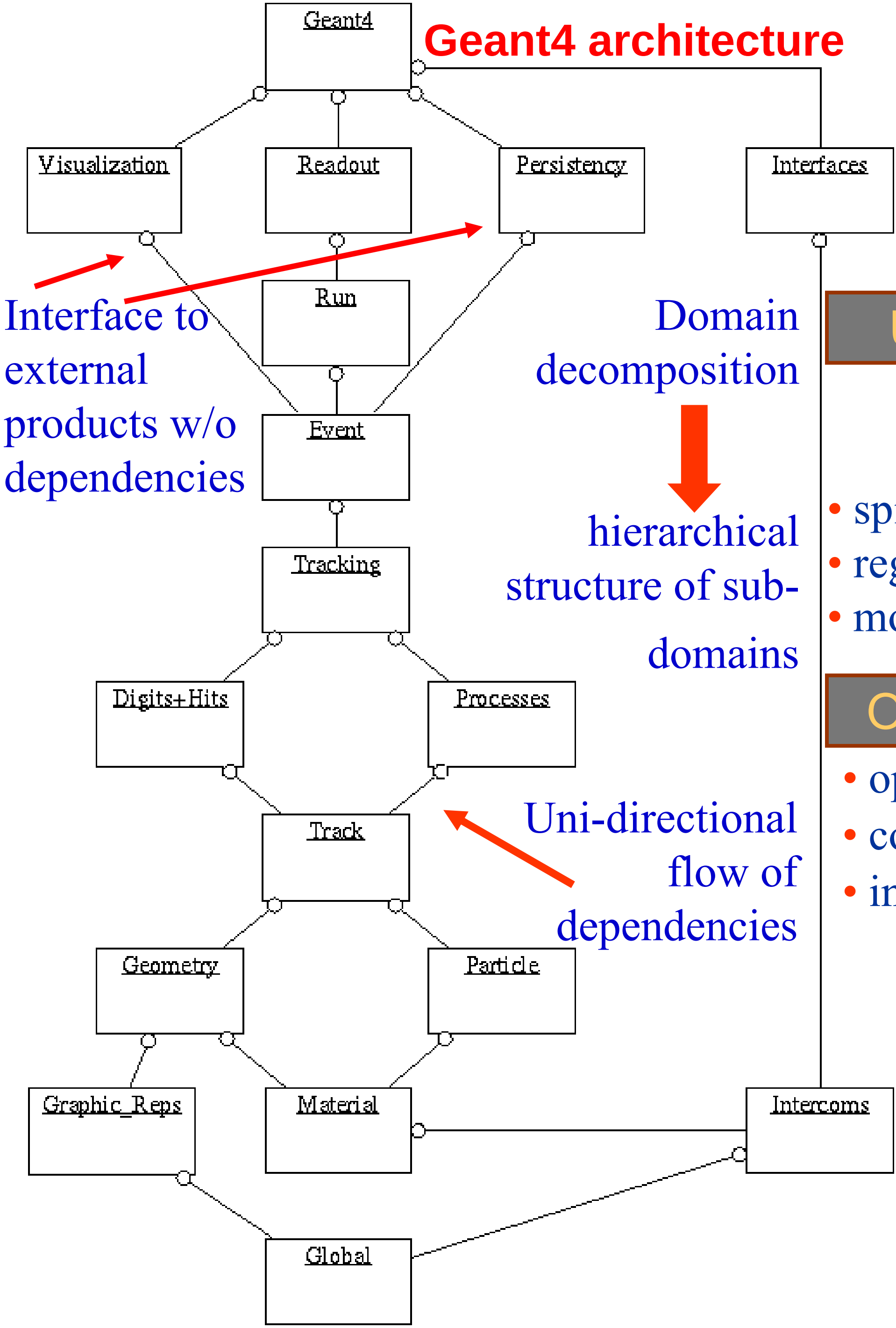
What characterizes Geant4

Or: the fundamental concepts, which all the rest is built upon

Physics

From the Minutes of LCB (LHCC Computing Board) meeting on 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."



Software Engineering

plays a fundamental role in Geant4

User Requirements

- formally collected
- systematically updated
- PSS-05 standard

Software Process

- spiral iterative approach
- regular assessments and improvements (SPI process)
- monitored following the ISO 15504 model

Object Oriented methods

- OOAD
- use of CASE tools
- openness to extension and evolution
- contribute to the transparency of physics
- interface to external software without dependencies

Quality Assurance

- commercial tools
- code inspections
- automatic checks of coding guidelines
- testing procedures at unit and integration level
- dedicated testing team

Use of Standards

- de jure and de facto

The functionality

What Geant4 can do
How well it does it

The kernel

Run and event

- Multiple events
  - possibility to handle the pile-up
- Multiple runs in the same job
  - with different geometries, materials etc.
- Powerful stacking mechanism
  - three levels by default: handle trigger studies, loopers etc.

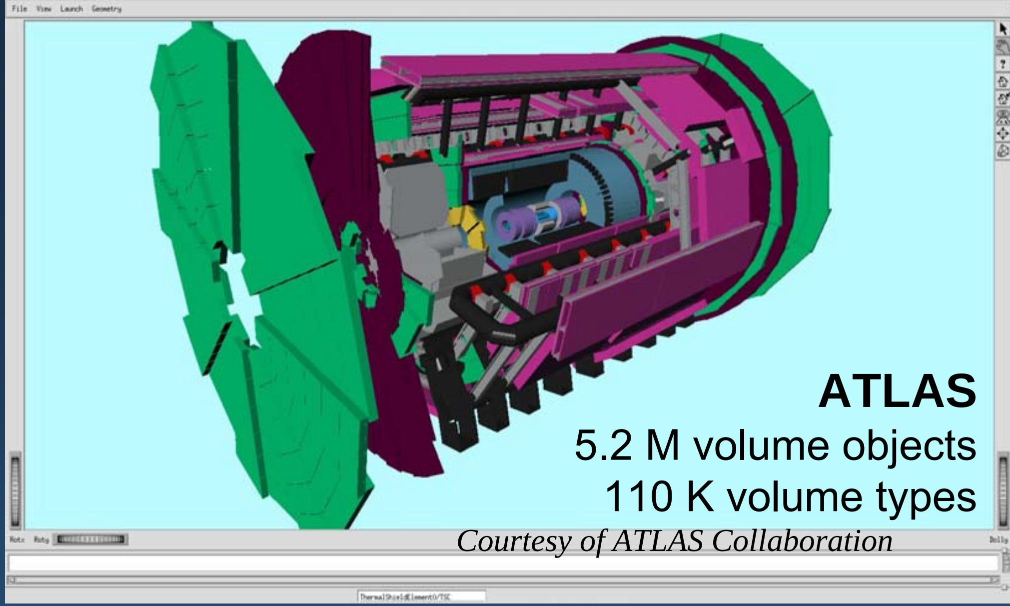
Tracking

- Decoupled from physics
  - all processes handled through the same abstract interface
- Independent from particle type
- New physics processes can be added to the toolkit without affecting tracking

Geant4 has only production thresholds, **no tracking cuts**

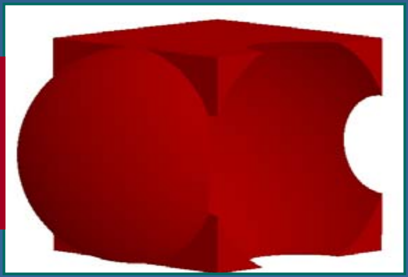
- all particles are tracked down to zero range
- energy, TOF ... cuts can be defined by the user

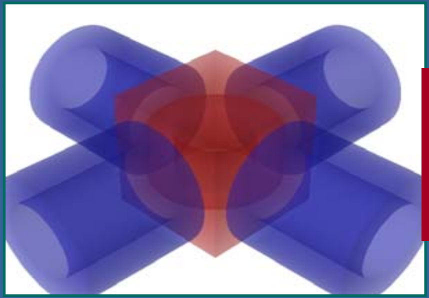
Geometry



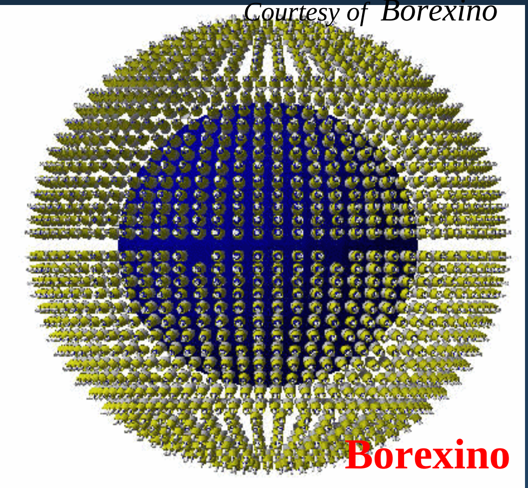
- Role
  - detailed detector description
  - efficient navigation
- Three conceptual layers
  - Solid: shape, size
  - LogicalVolume: material, sensitivity, daughter volumes, etc.
  - PhysicalVolume: position, rotation
- One can do fancy things with geometry…

Boolean operations

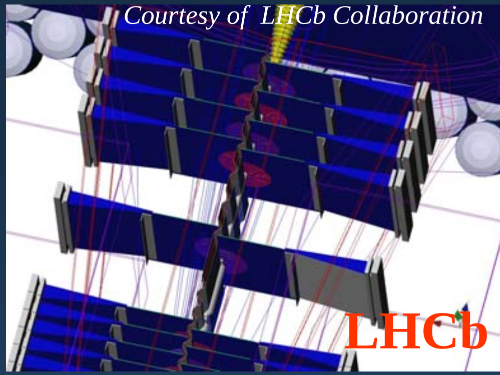




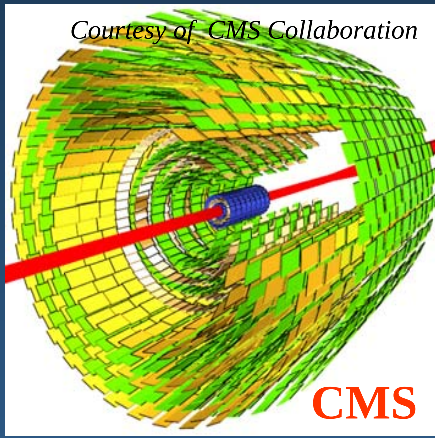
Transparent solids

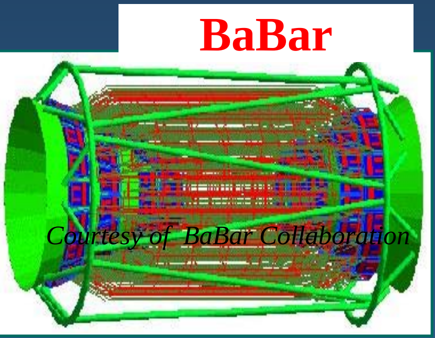


Solids

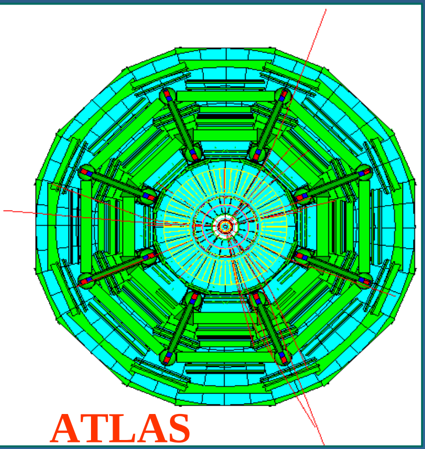


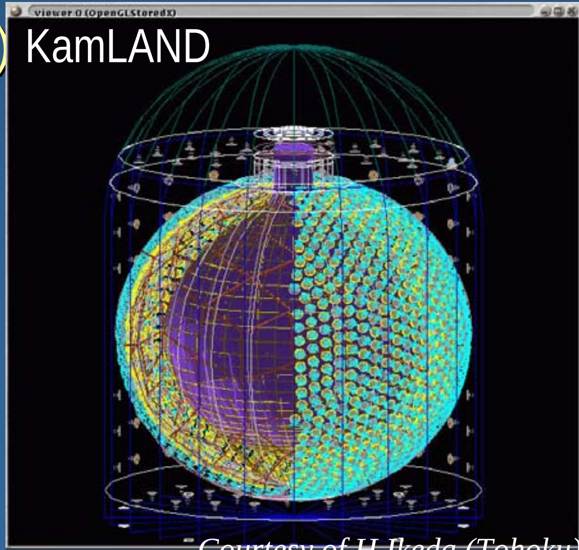
Multiple representations
Same abstract interface





- CSG (**C**onstructed **S**olid **G**eometries)
  - simple solids
- STEP extensions
  - polyhedra, spheres, cylinders, cones, toroids, etc.
- BREPS (**B**oundary **REP**resented **S**olids)
  - volumes defined by boundary surfaces
  - include solids defined by NURBS *(Non-Uniform Rational B-Splines)*

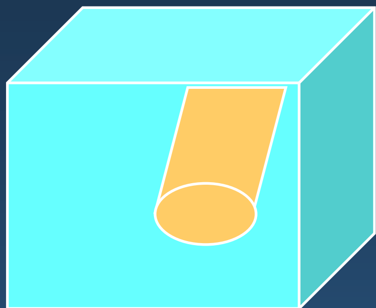




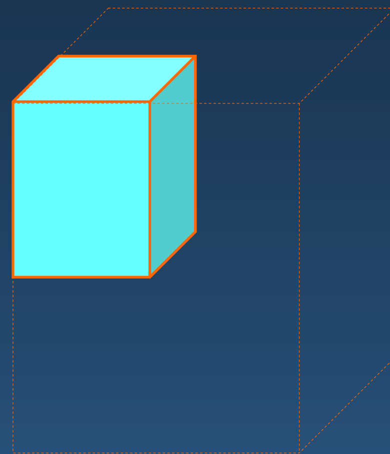
Courtesy of H.Ikeda (Tohoku)

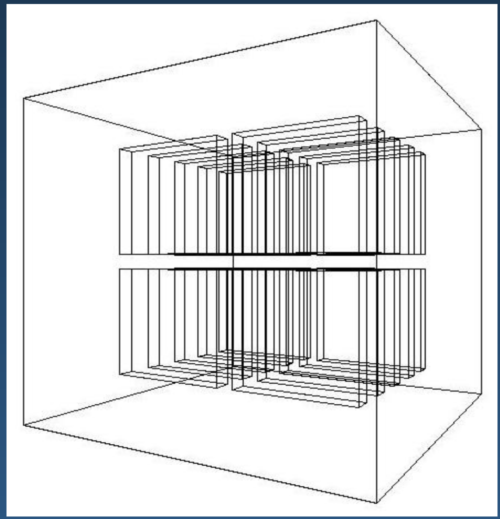
CAD exchange: ISO STEP interface

Physical Volumes

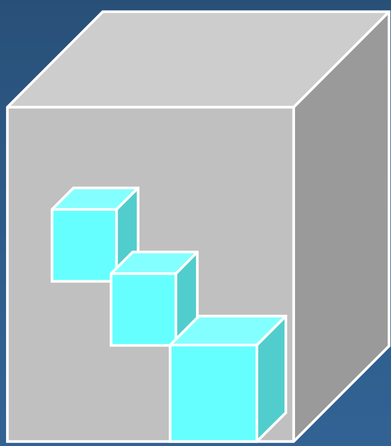


placement

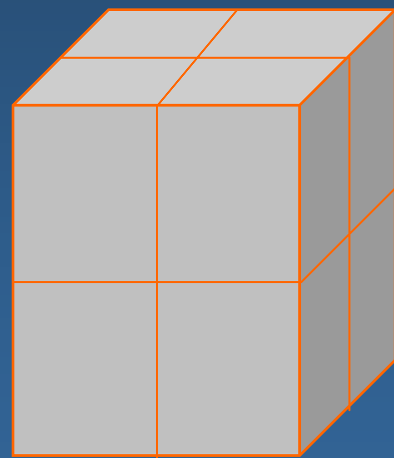




assembled



parameterised

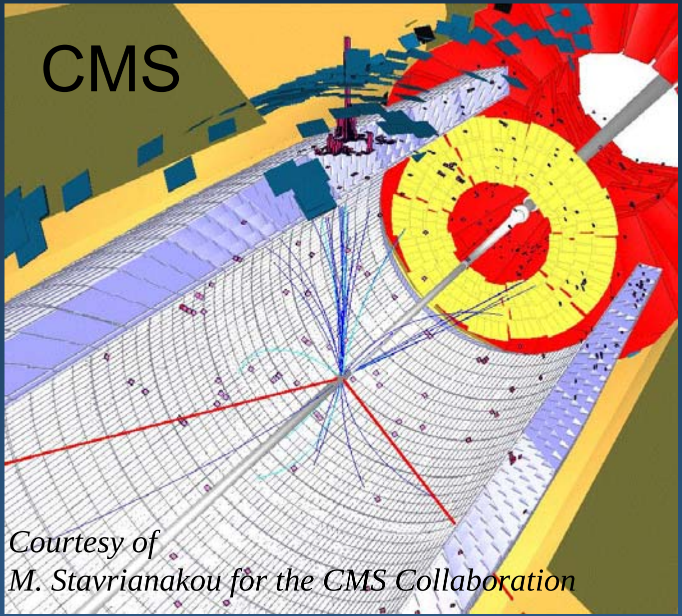


replica

Versatility to describe complex geometries

Electric and magnetic fields

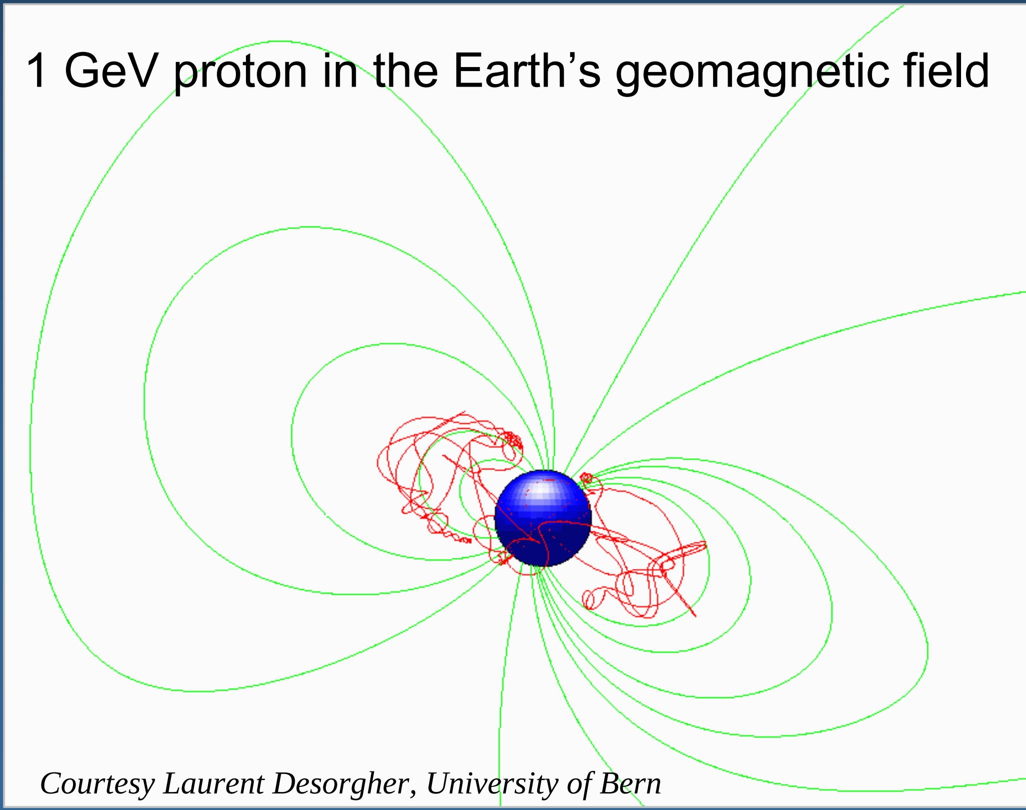
of variable non-uniformity and differentiability



Courtesy of M. Stavrianakou for the CMS Collaboration

Geant4 field ~ 2 times faster than FORTRAN/GEANT3

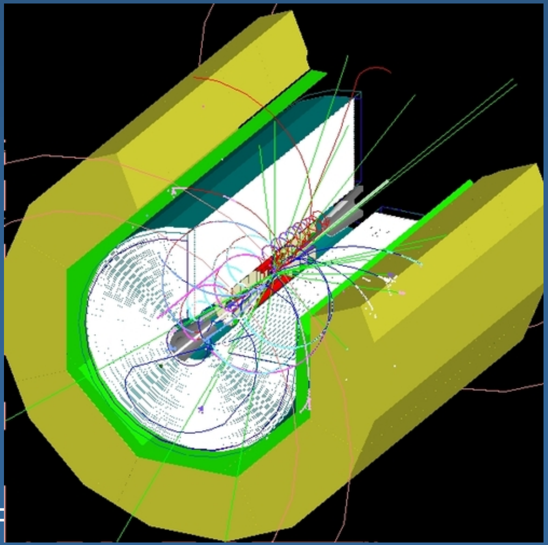
1 GeV proton in the Earth's geomagnetic field



Courtesy Laurent Desorgher, University of Bern

MOKKA

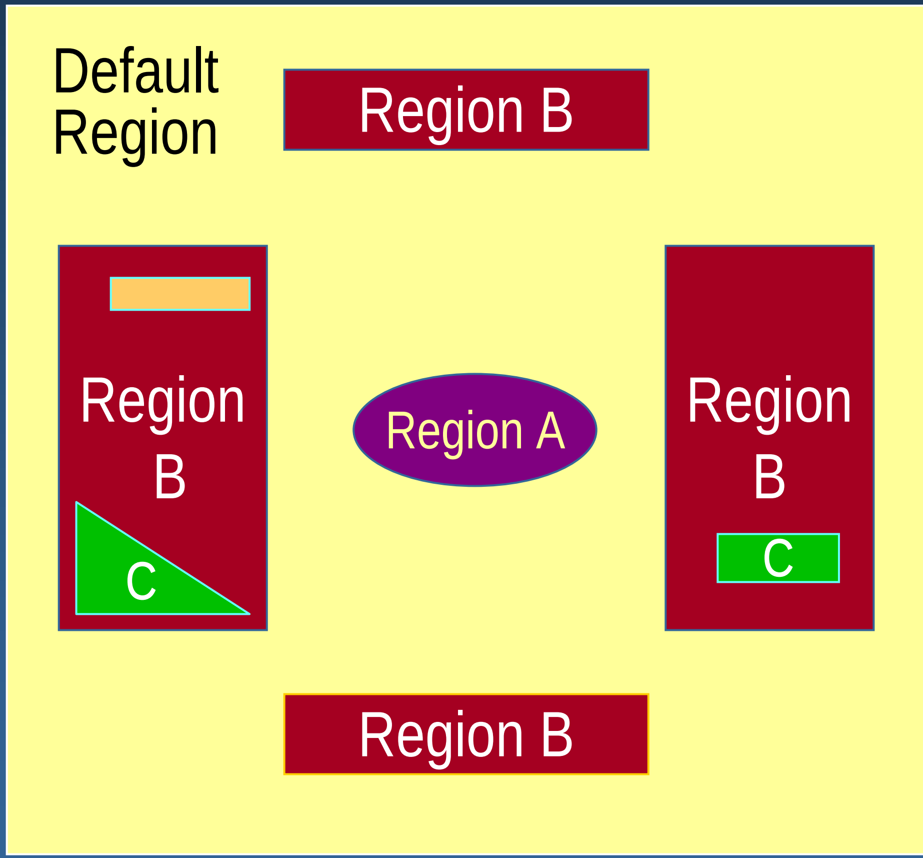
Linear Collider Detector

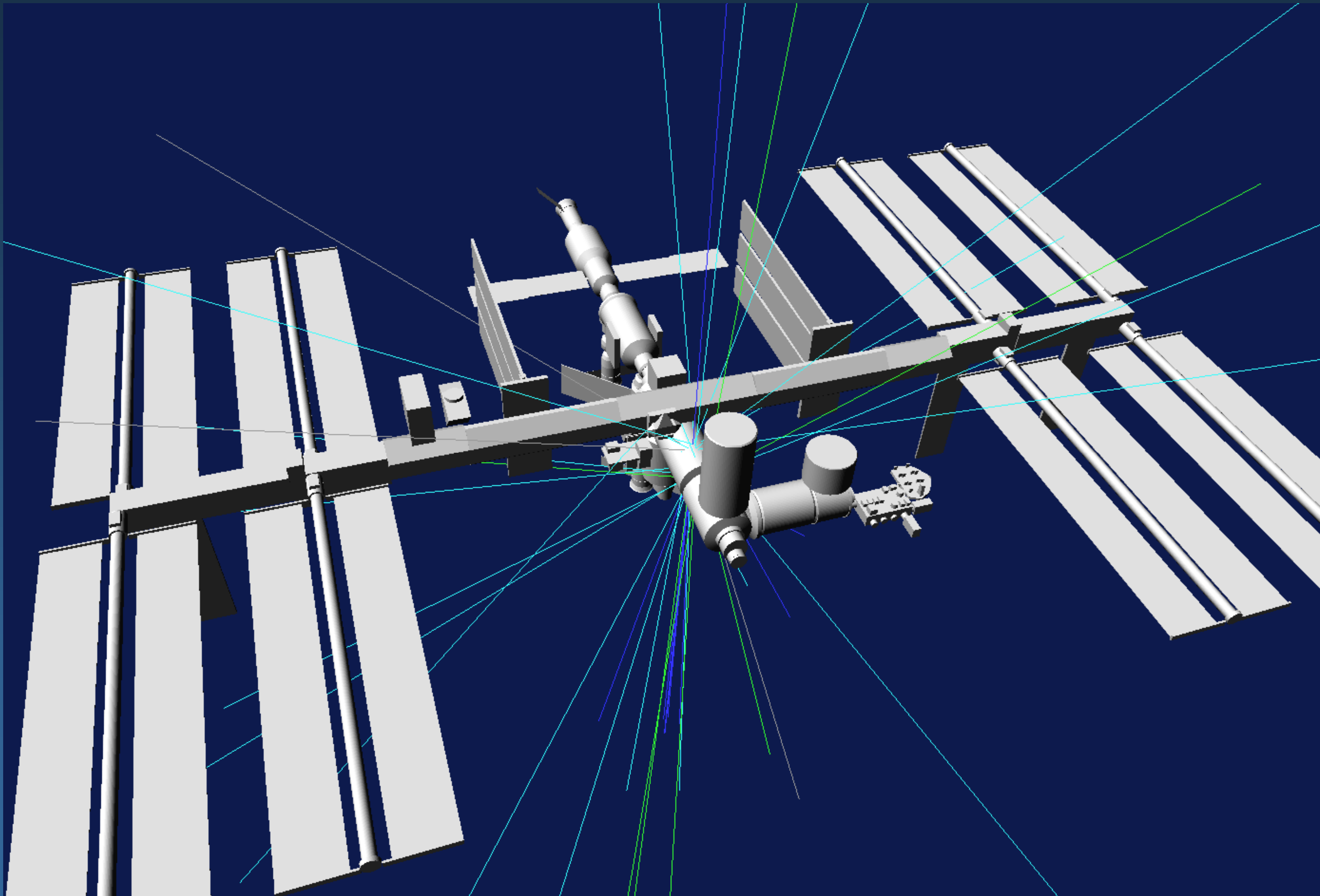


Detector Region

- Concept of region:
  - Set of geometry volumes
    - barrel + end-caps of the calorimeter
    - support structures
    - etc.
  - Or any group of volumes

- A set of cuts in range is associated to a region
  - a different cut for each particle is allowed in a region

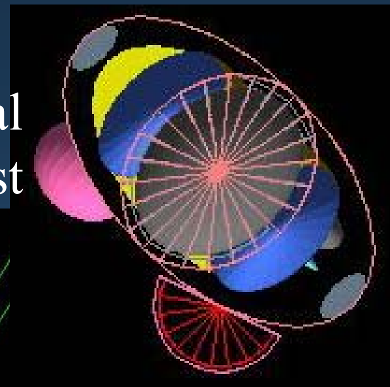




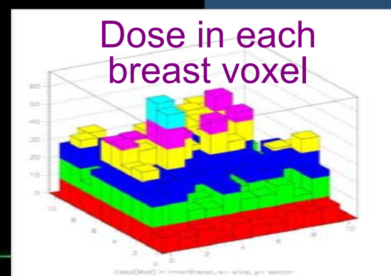
Courtesy T. Ersmark, KTH Stockholm

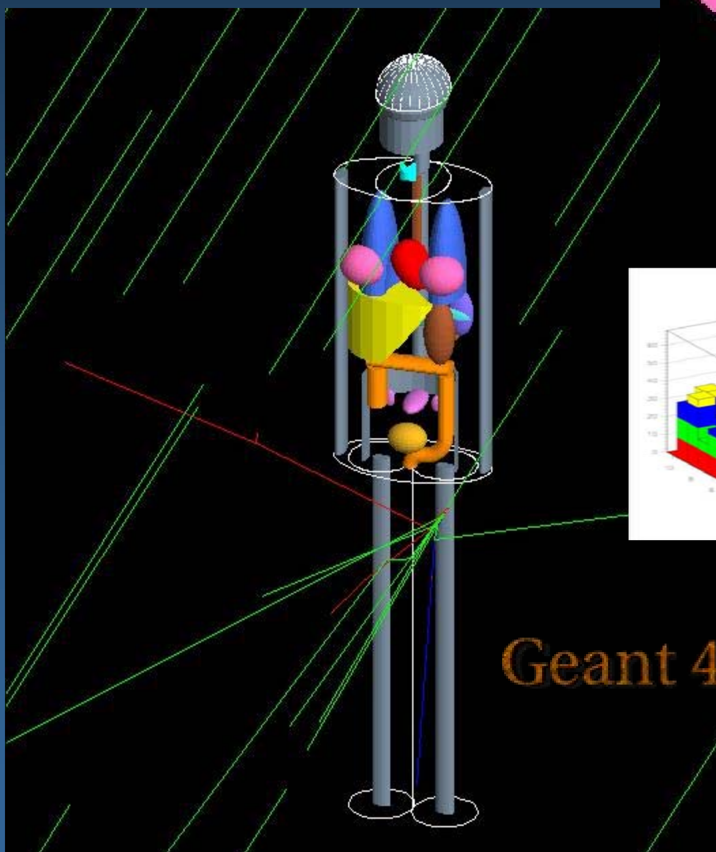
Not only large scale, complex detectors….

Analytical breast breast

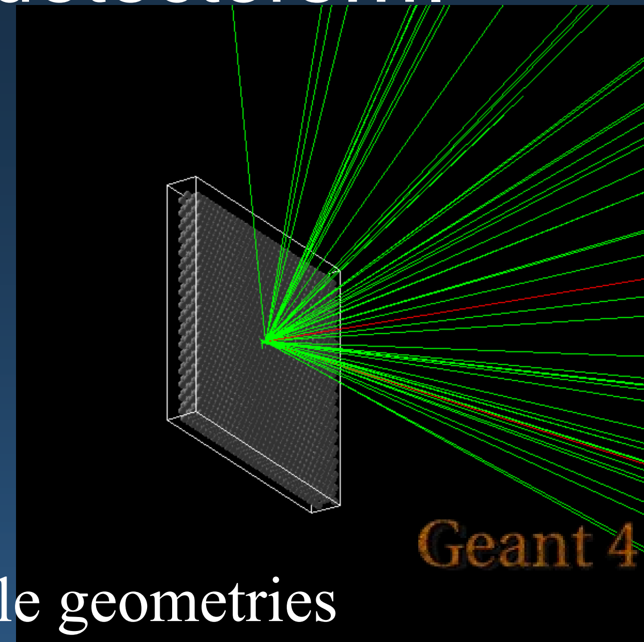


Voxel breast



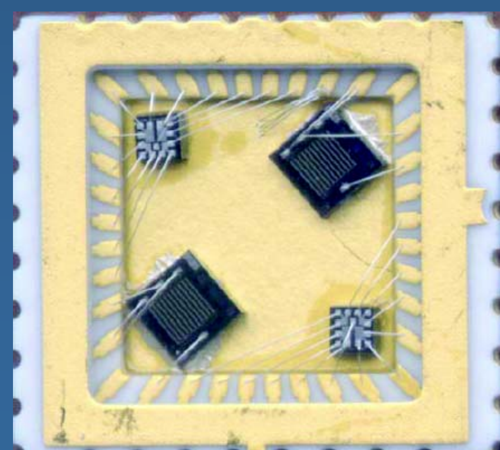


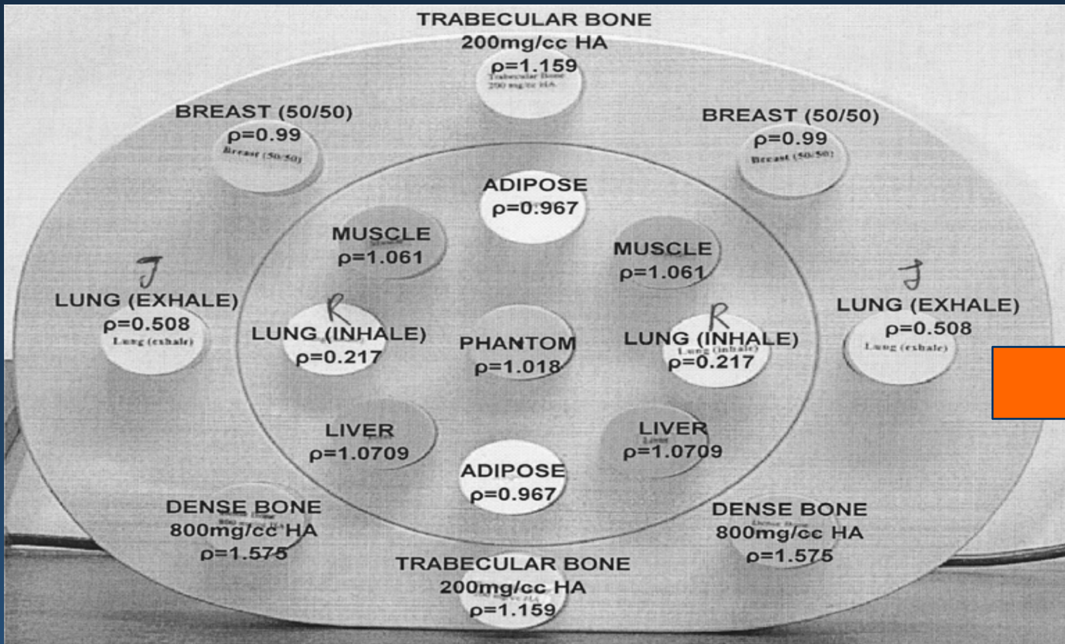
Geant4 anthropomorphic phantoms

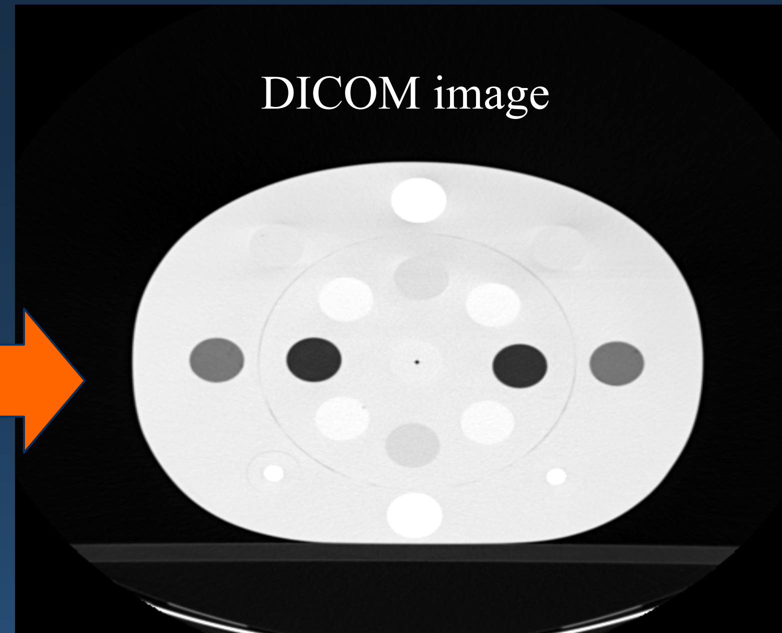


simple geometries

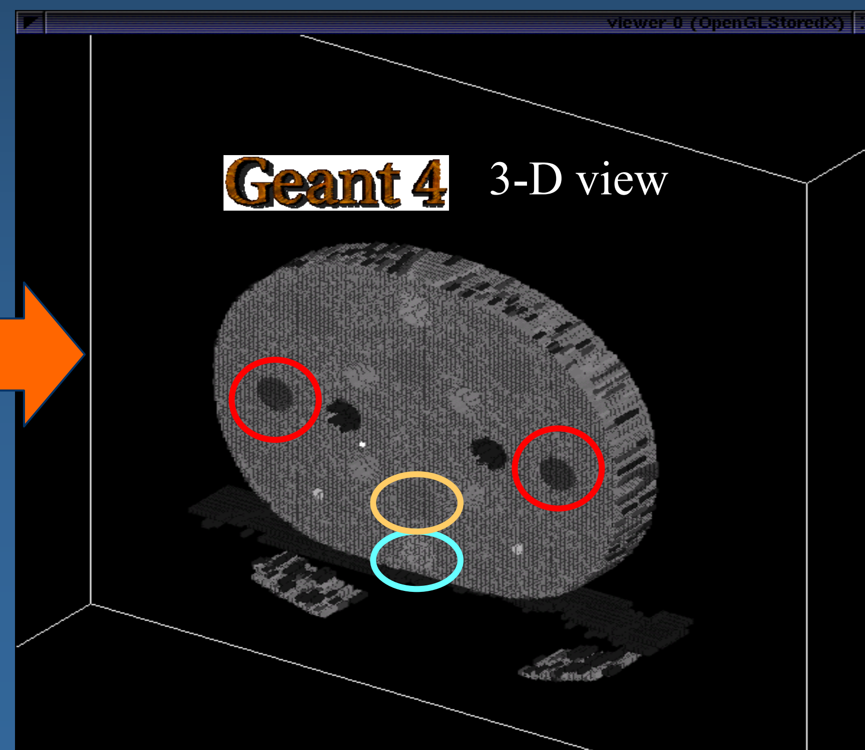
small scale components





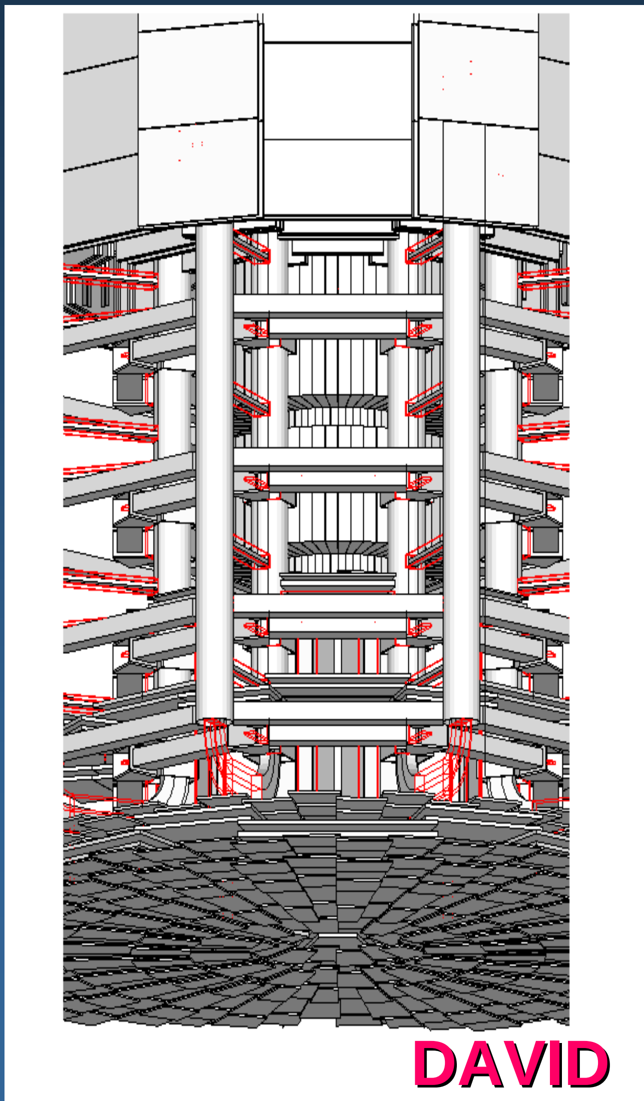


- Reading image information
- Transformation of pixel data into densities
- Association of densities to a list of materials
- Defining the voxels
  - Geant4 parameterised volumes
  - parameterisation function: material

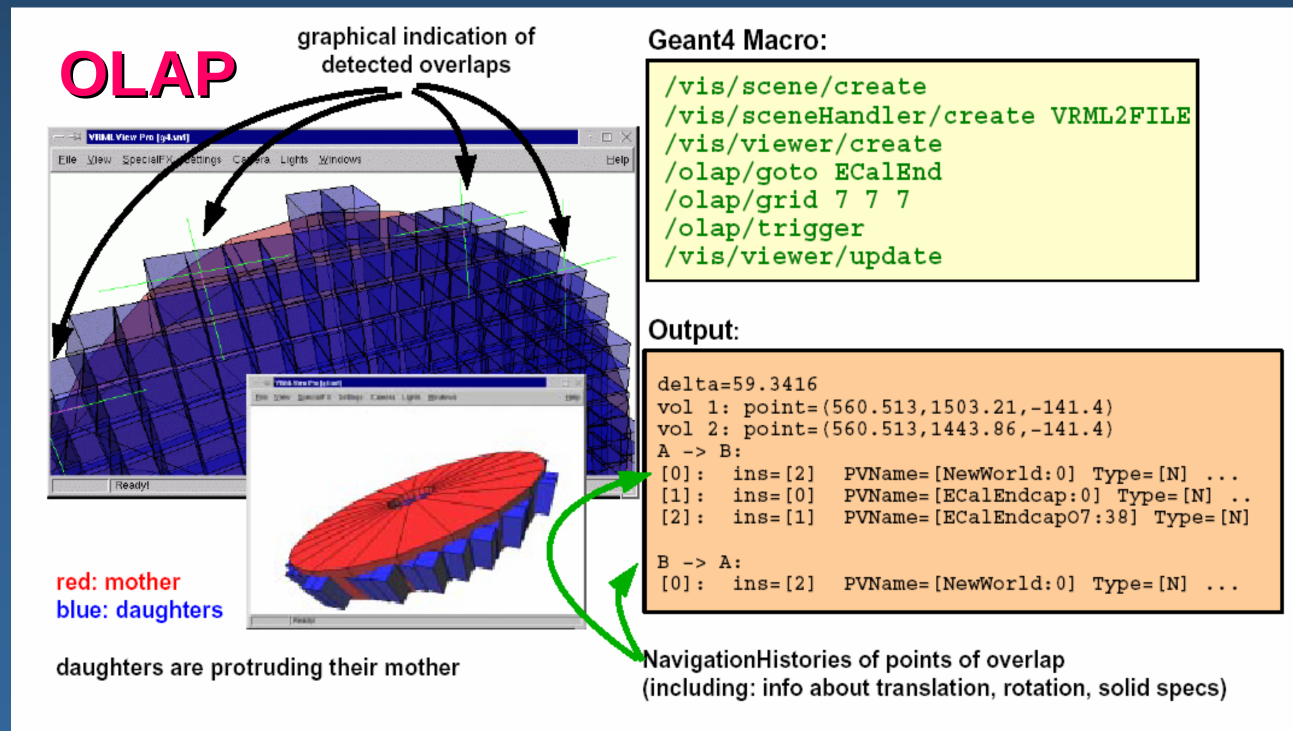


CENTRE DE RECHERCHE
Pavillon L'Hôtel-Dieu
Centre hospitalier universitaire de Québec
UNIVERSITÉ LAVAL
L. Archambault, L. Beaulieu,
V.-H. Tremblay

You may also do it wrong…



Tools to detect badly defined geometries



Physics

- Abstract interface to physics processes
  - **Tracking independent from physics**
  - Uniform treatment of electromagnetic and hadronic processes

- Distinction between **processes** and **models**
  - multiple models for the same physics process *(complementary/alternative)*

- Transparency (supported by *encapsulation* and *polymorphism*)
  - Calculation of cross-sections independent from the way they are accessed (data files, analytical formulae etc.)
  - Calculation of the final state independent from tracking

- Explicit use of units throughout the code

- Open system
  - Users can easily create and use their own models

Data libraries

- Systematic collection and evaluation of experimental data from many sources worldwide
- Databases
  - ENDF/B, JENDL, FENDL, CENDL, ENSDF,JEF, BROND, EFF, MENDL, IRDF, SAID, EPDL, EEDL, EADL, SANDIA, ICRU etc.
- Collaborating distribution centres
  - NEA, LLNL, BNL, KEK, IAEA, IHEP, TRIUMF, FNAL, Helsinki, Durham etc.
- The use of evaluated data is important for the validation of physics results of the experiments

46

Electromagnetic physics

- electrons and positrons
- γ, X-ray and optical photons
- muons
- charged hadrons
- ions

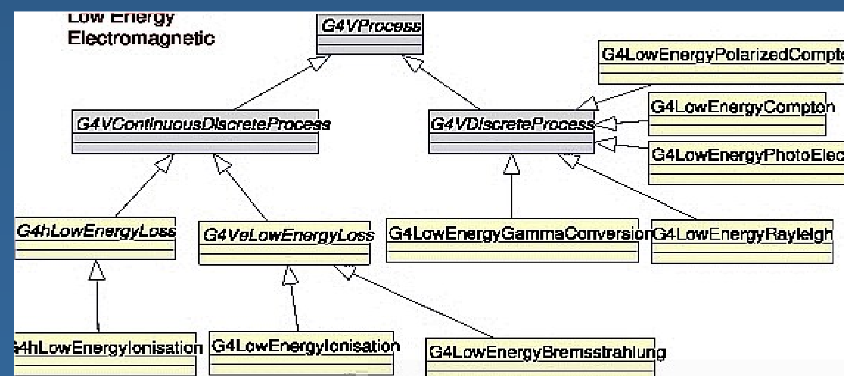
Comparable to Geant3 already in the α release (1997)

Further extensions *(facilitated by the OO technology)*

energy loss {

- Multiple scattering
- Bremsstrahlung
- Ionisation
- Annihilation
- Photoelectric effect
- Compton scattering
- Rayleigh effect
- γ conversion
- e^+e^- pair production
- Synchrotron radiation
- Transition radiation
- Cherenkov
- Refraction
- Reflection
- Absorption
- Scintillation
- Fluorescence
- Auger

- High energy extensions
  - needed for LHC experiments, cosmic ray experiments…
- Low energy extensions
  - fundamental for space and medical applications, dark matter and ν experiments, antimatter spectroscopy etc.
- Alternative models for the same process



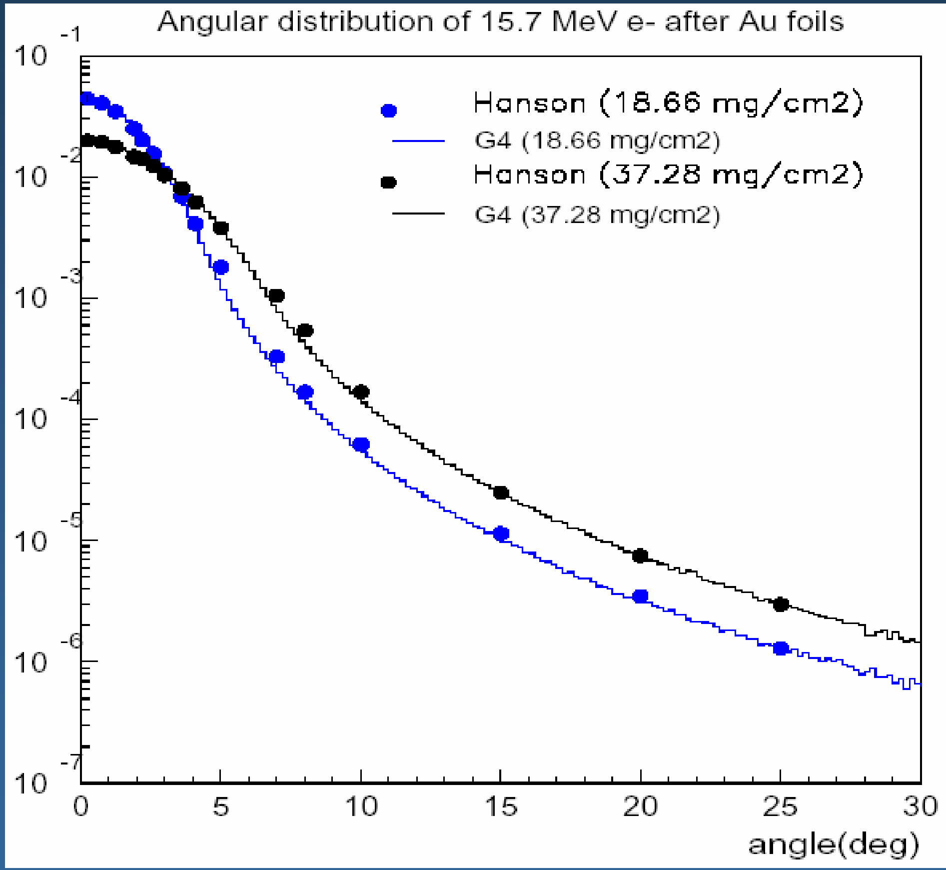
All obeying to the same abstract Process interface → transparent to tracking

Standard electromagnetic processes

1 keV up to O(100 TeV)

- Multiple scattering
  - model based on Lewis theory
  - computes mean free path length and lateral displacement
- New energy loss algorithm
  - optimises the generation of δ rays near boundaries
- Variety of models for ionisation and energy loss
  - including PhotoAbsorption Interaction model (for thin layers)
- Many optimised features
  - Secondaries produced only when needed
  - Sub-threshold production

Multiple scattering



MuScat (TRIUMF E875)

- Multiple scattering of muons of momenta up to 200 MeV/c
- Important for the optimal design of a cooling channel for a ν factory or μ collider

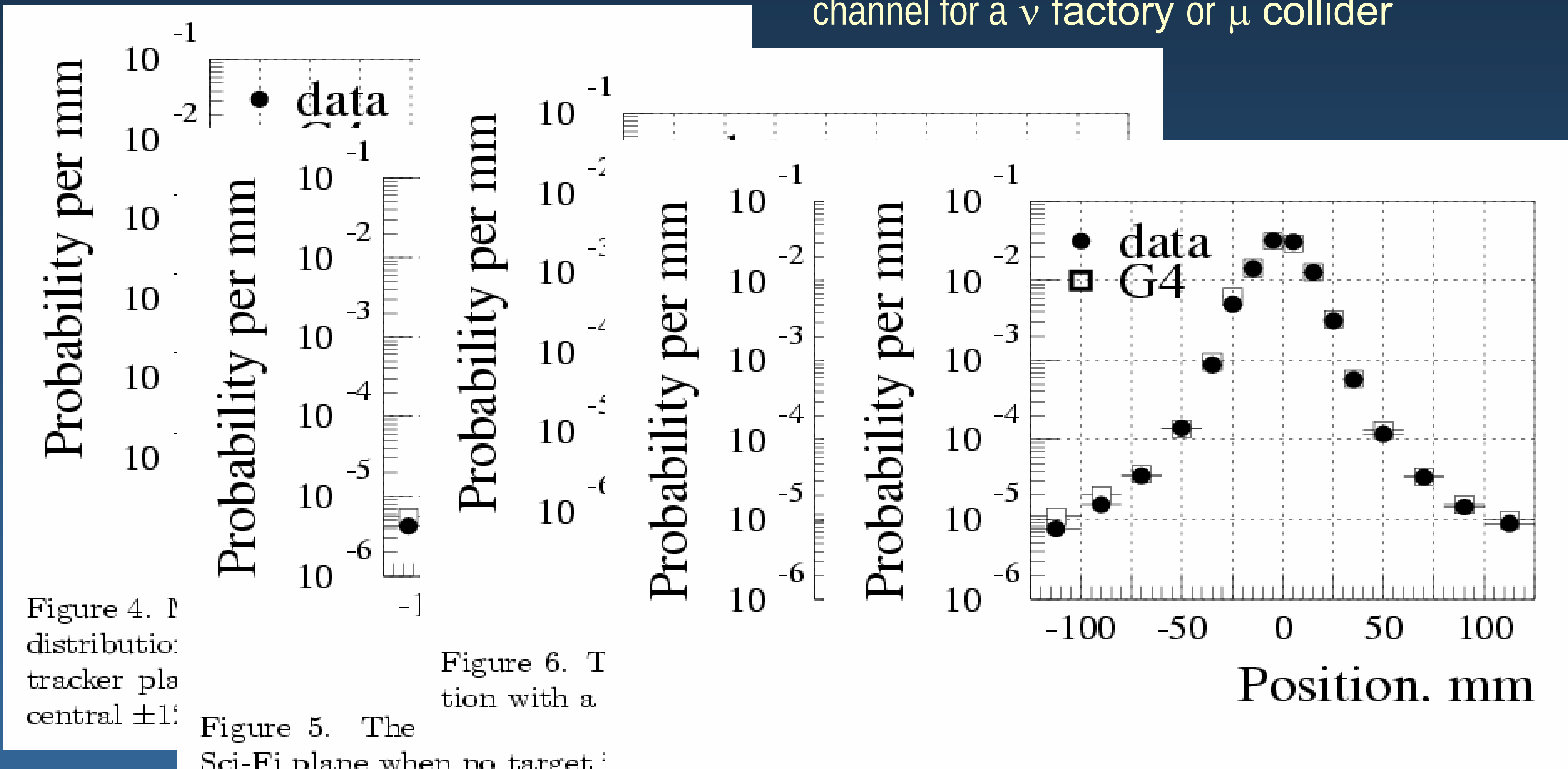


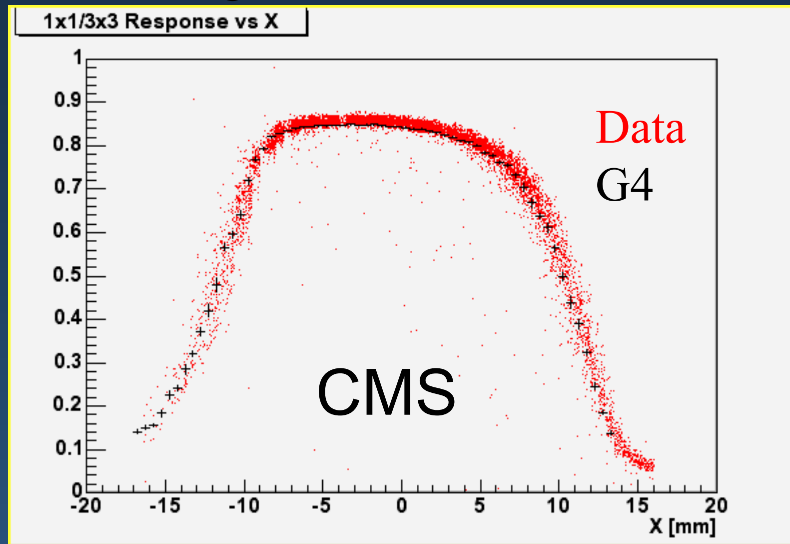
Figure 7. The
tion with a 3.

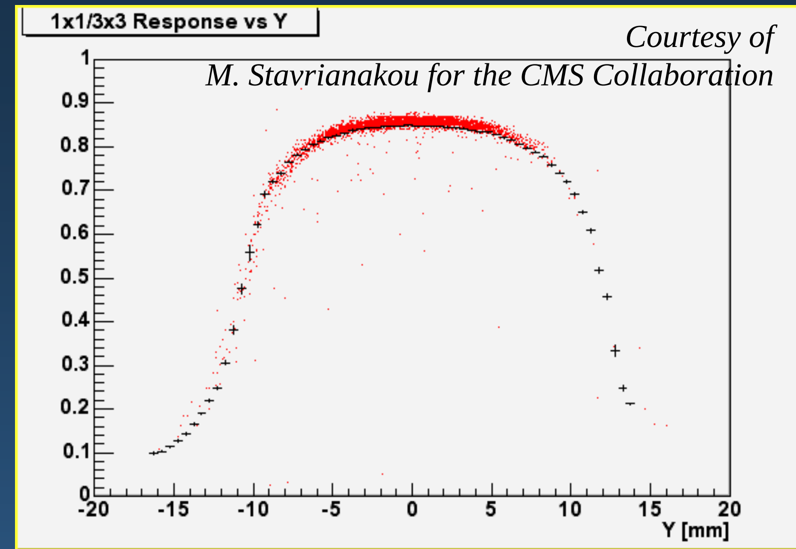
Figure 8. The measured and simulated arrival position distributions with a 150 mm liquid hydrogen target.

Courtesy of W.J. Murray (RAL)

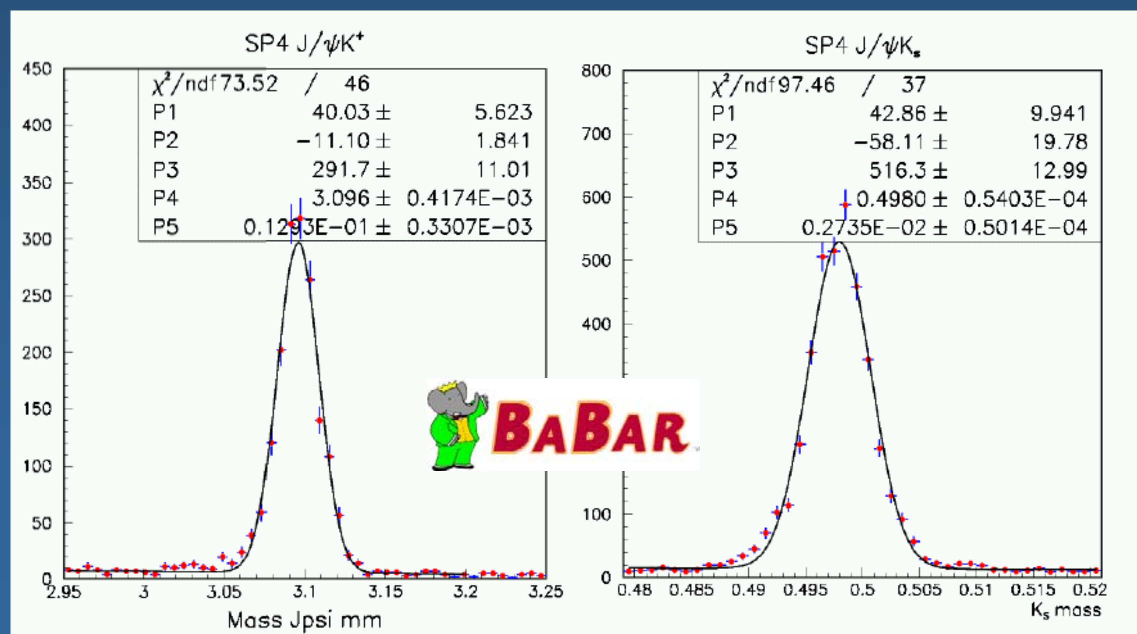
Calorimetry

Single crystal containment: E_{1x1}/E_{3x3} versus position

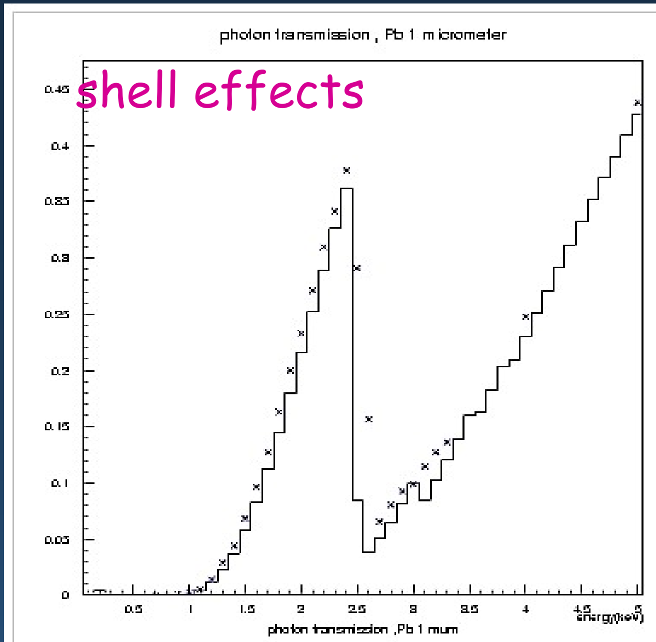




Tracking



Geant4 Standard Electromagnetic Physics



Geant 4

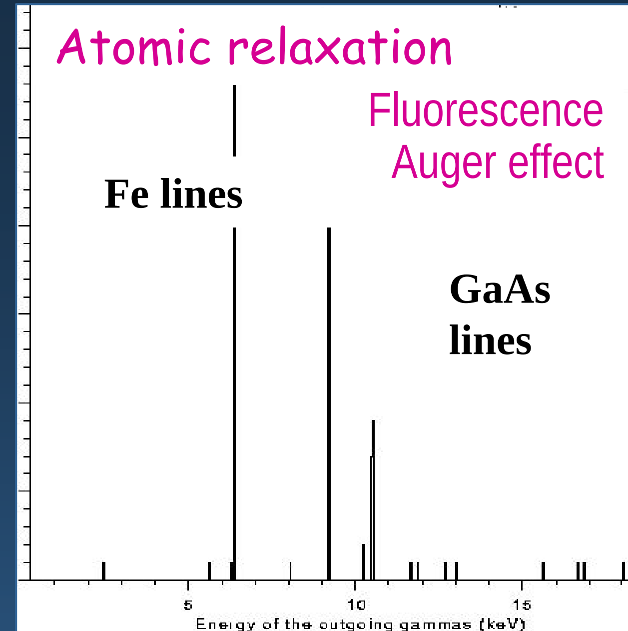
e,γ down to 250/100 eV

EGS4, ITS to 1 keV

Geant3 to 10 keV

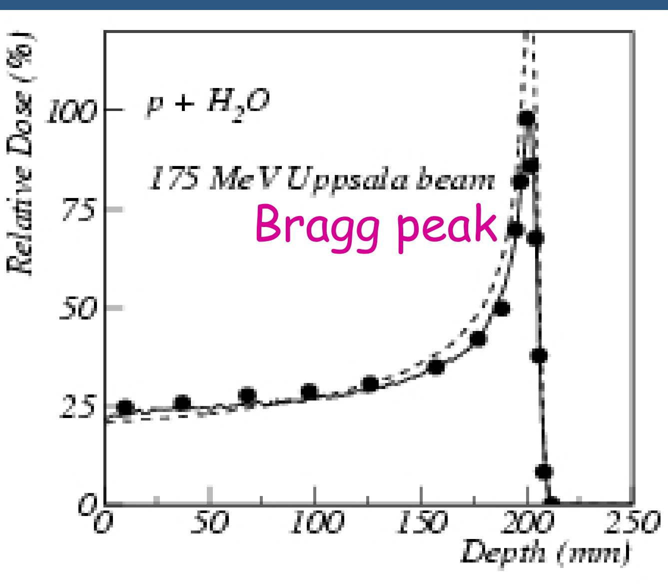
① Based on EPDL97, EEDL and EADL evaluated data libraries

② Based on Penelope analytical models



Hadron and ion models based on Ziegler and ICRU data and parameterisations

Barkas effect (charge dependence) models for **negative hadrons**



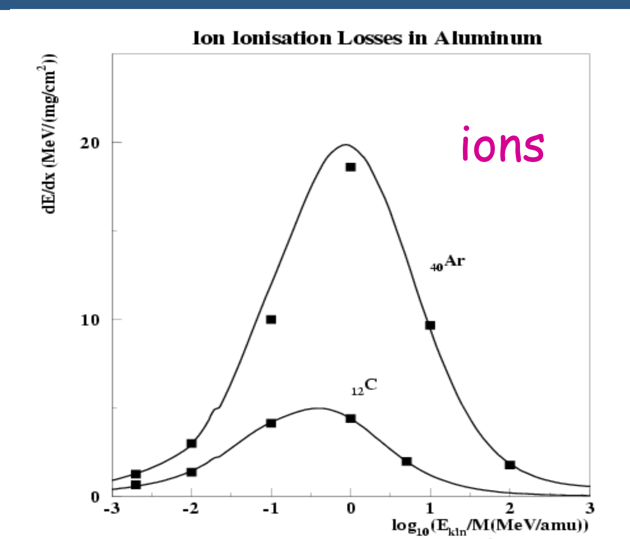
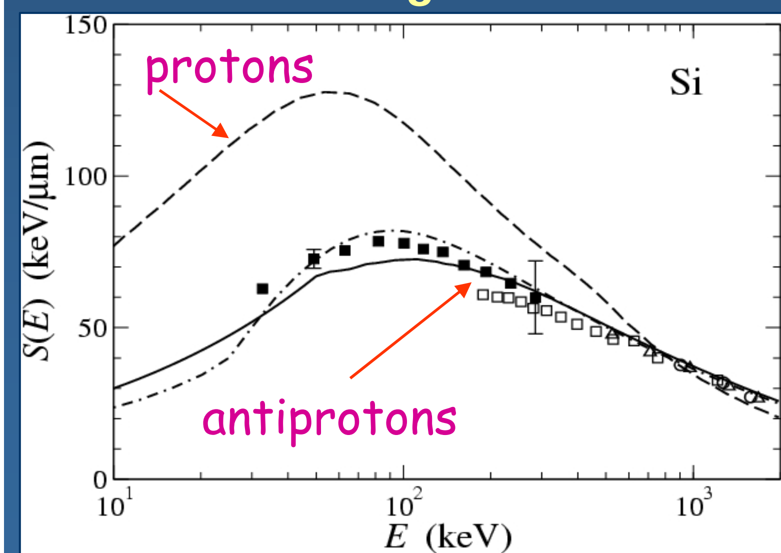


Figure 9: Ion electronic stopping power in aluminum. Points - the best fit on the data from Ref.[12], solid line - GEANT4 parameterisation. The accuracy of the data is about 5 %.



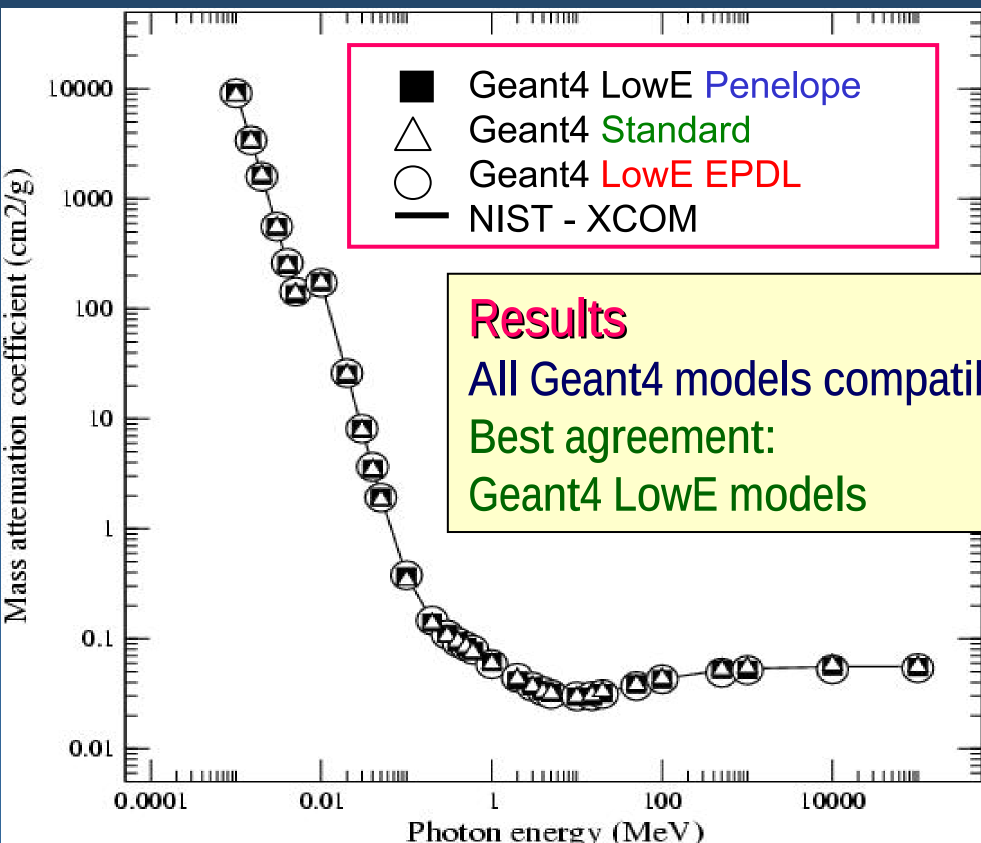
“Comparison of Geant4 electromagnetic physics models against the NIST reference data”

IEEE Transactions on Nuclear Science, vol. 52 (4), pp. 910-918, 2005

Geant4 electromagnetic physics models are accurate

Compatible with NIST data within NIST accuracy (LowE p-value > 0.9)

Mass attenuation coefficient in Fe

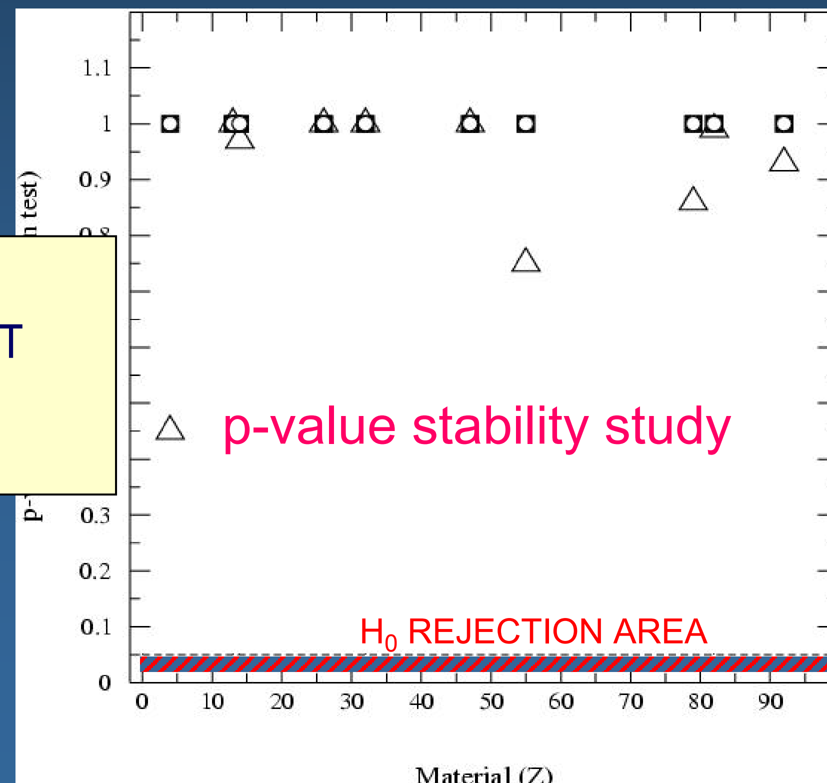


Results

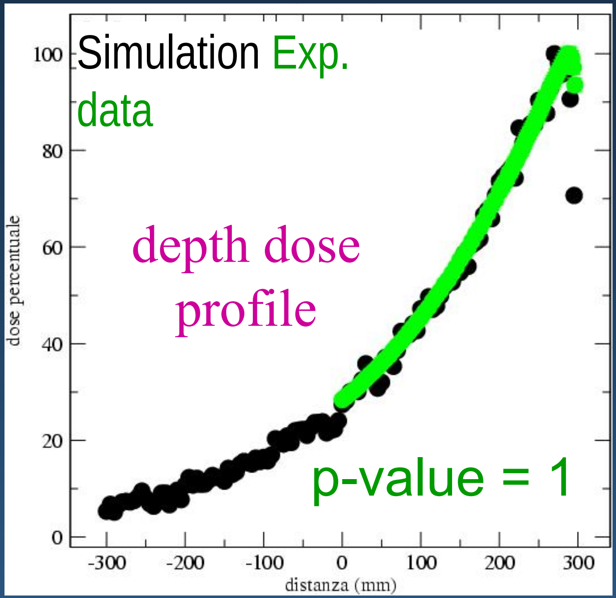
All Geant4 models compatible with NIST

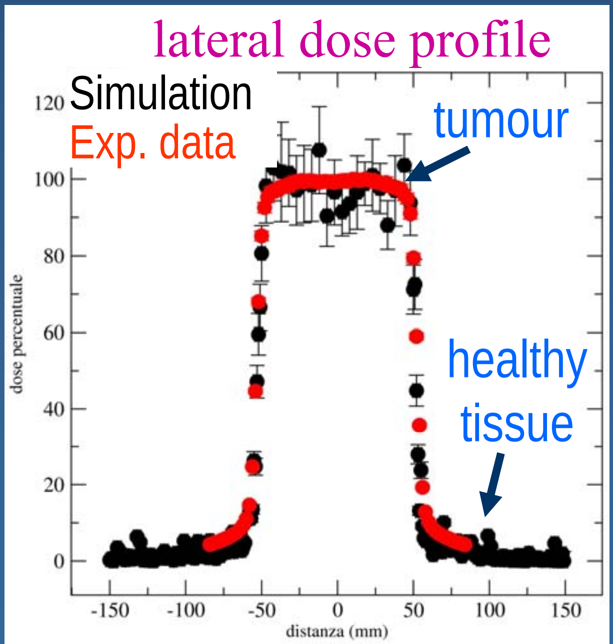
Best agreement:

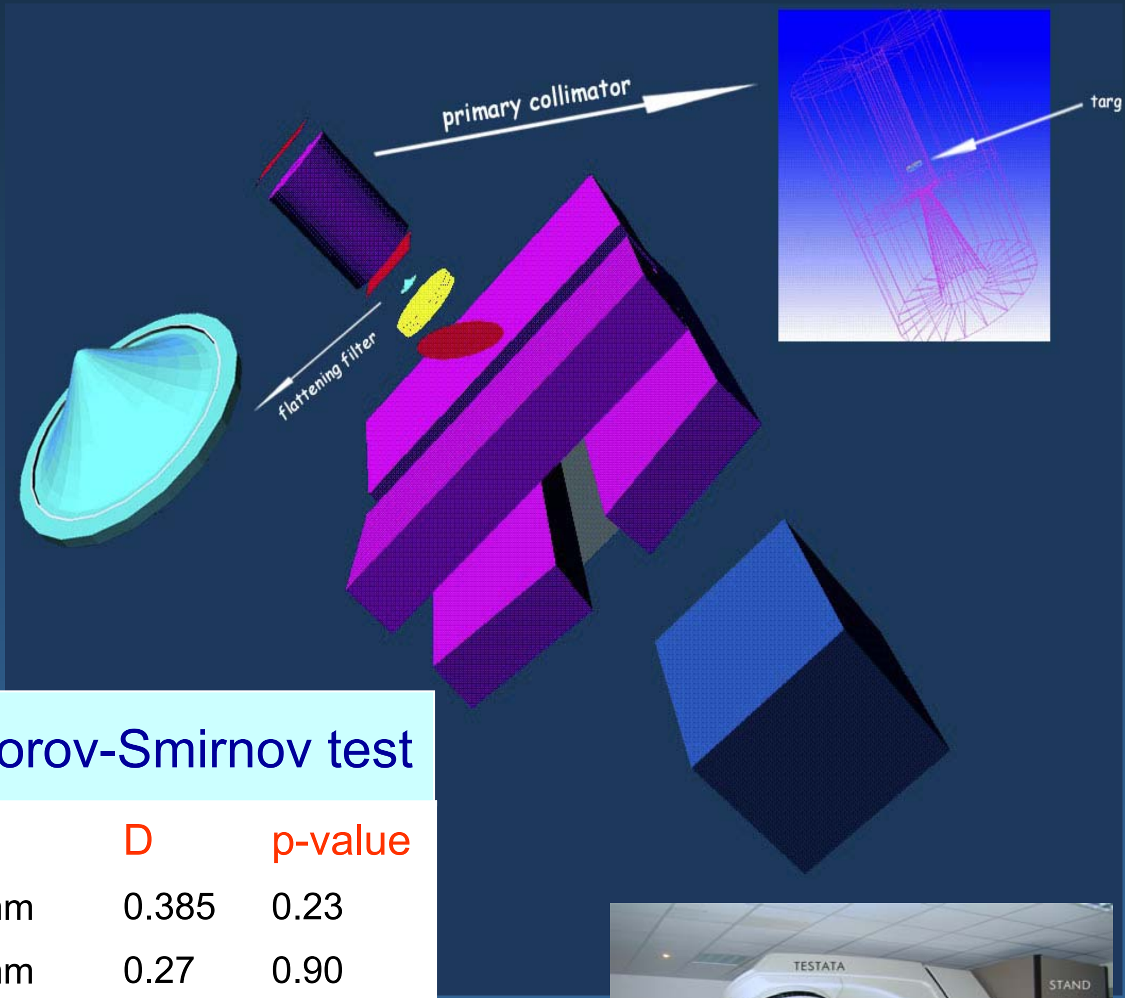
Geant4 LowE models



A medical accelerator for IMRT



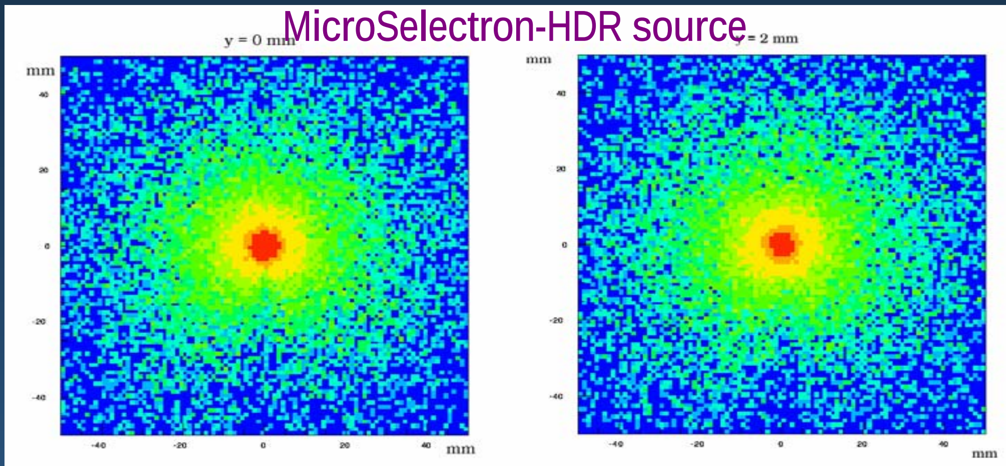




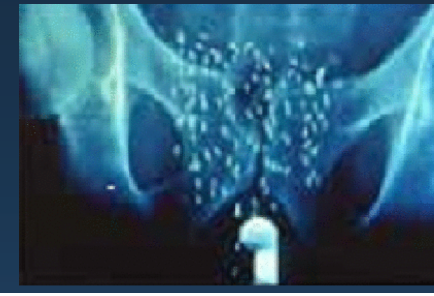
Kolmogorov-Smirnov test

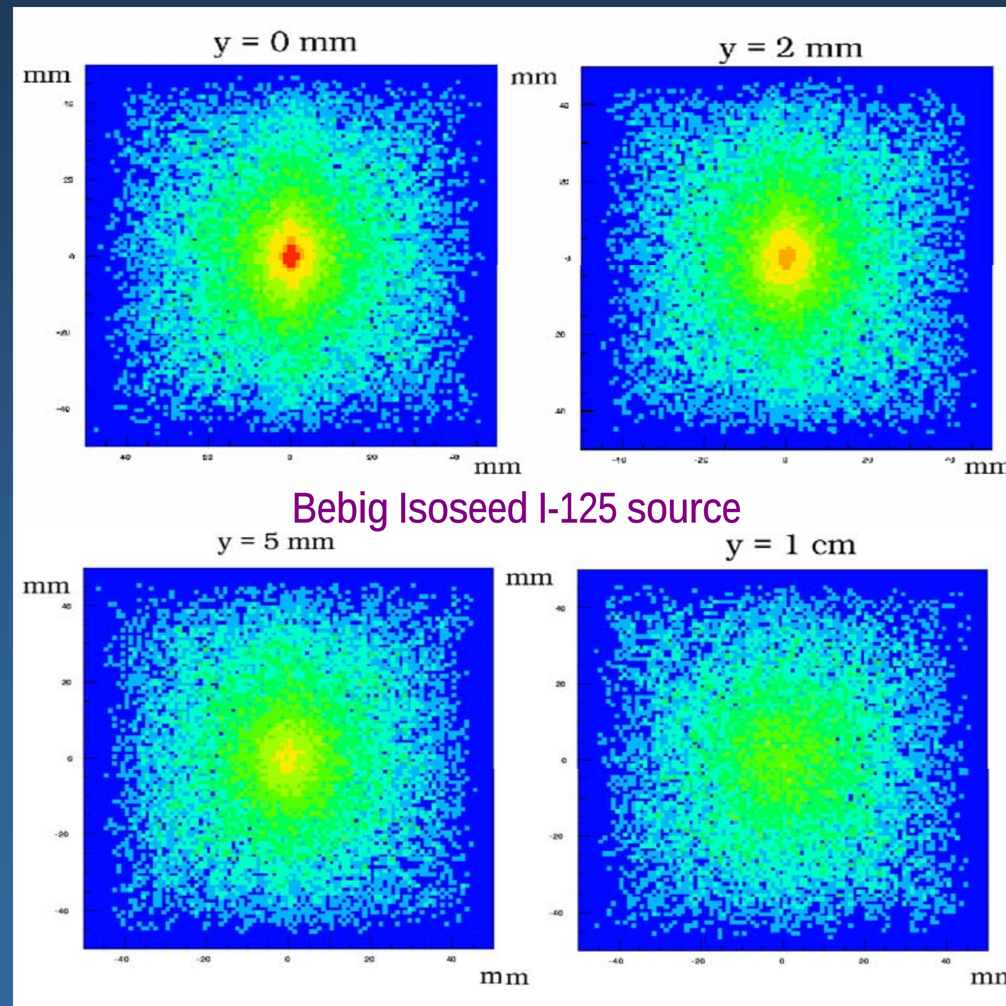
range	D	p-value
-84 ÷ -60 mm	0.385	0.23
-59 ÷ -48 mm	0.27	0.90
-47 ÷ 47 mm	0.43	0.19
48 ÷ 59 mm	0.30	0.82
60 ÷ 84 mm	0.40	0.10

Dosimetry
Endocavitary brachytherapy

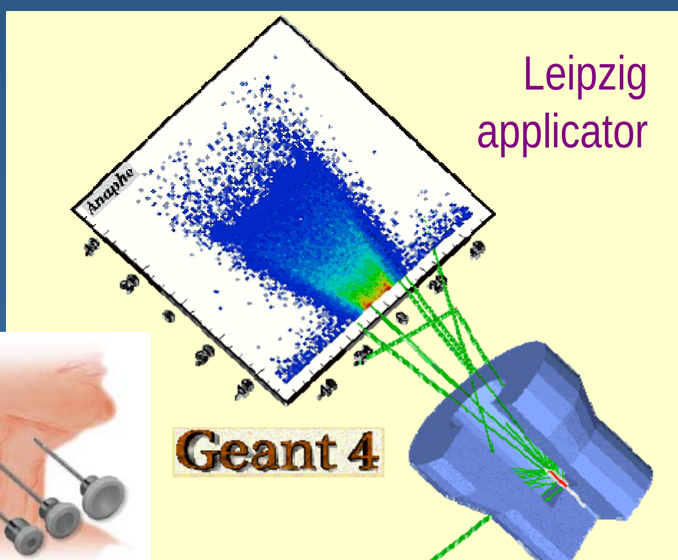


Dosimetry
Interstitial brachytherapy





Dosimetry
Superficial brachytherapy

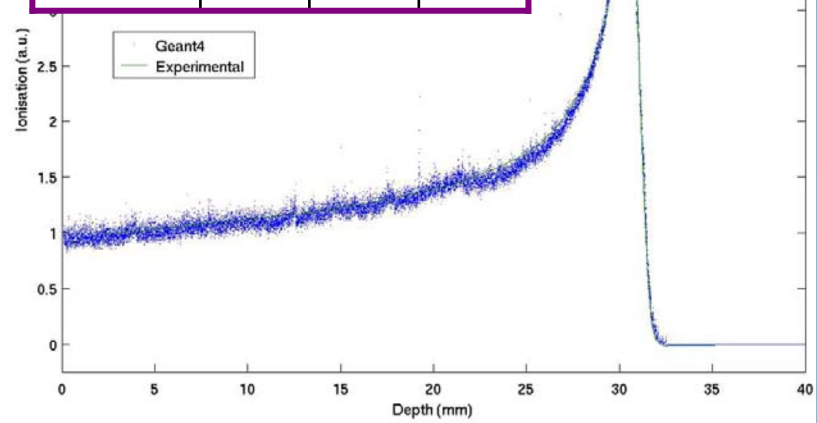


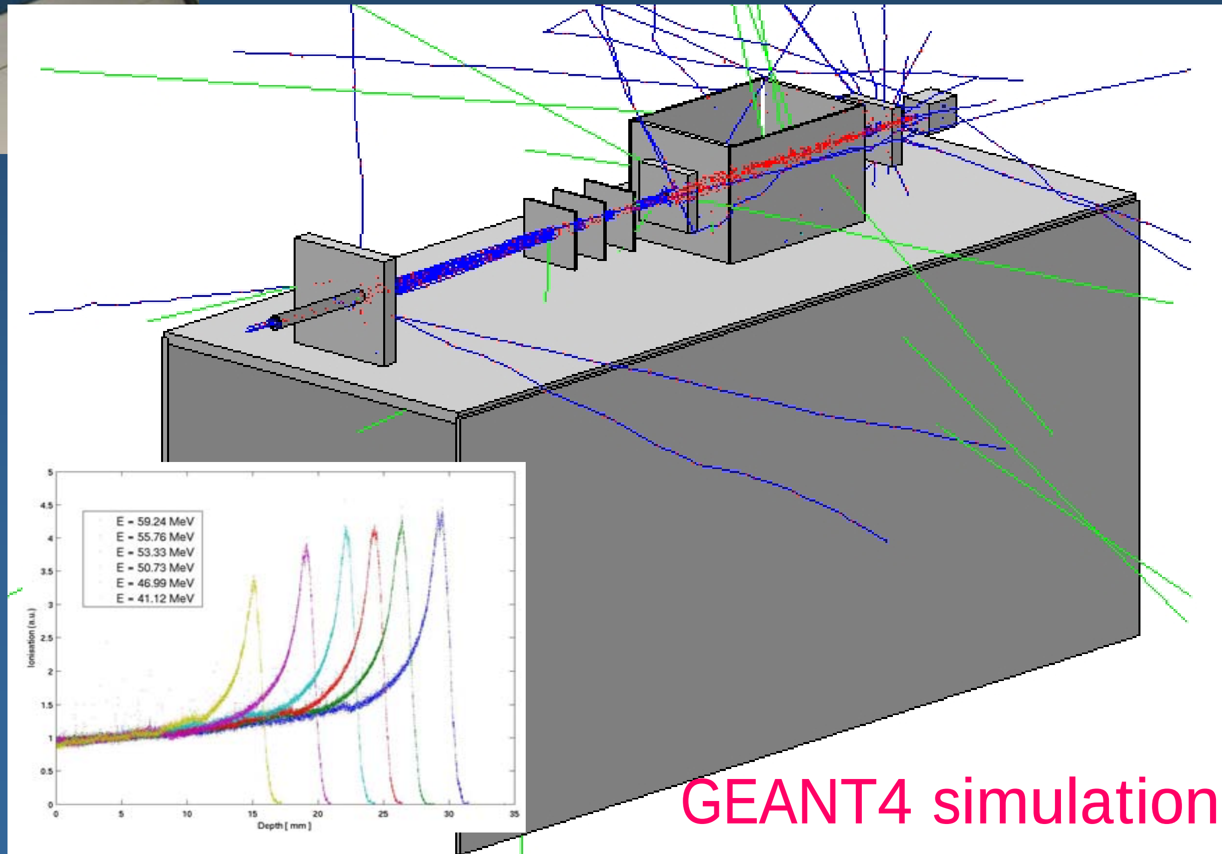
Real hadrontherapy beam line

CATANA hadrontherapy

Paper to be submitted to
IEEE Trans. Nucl. Sci., Dec. 2006

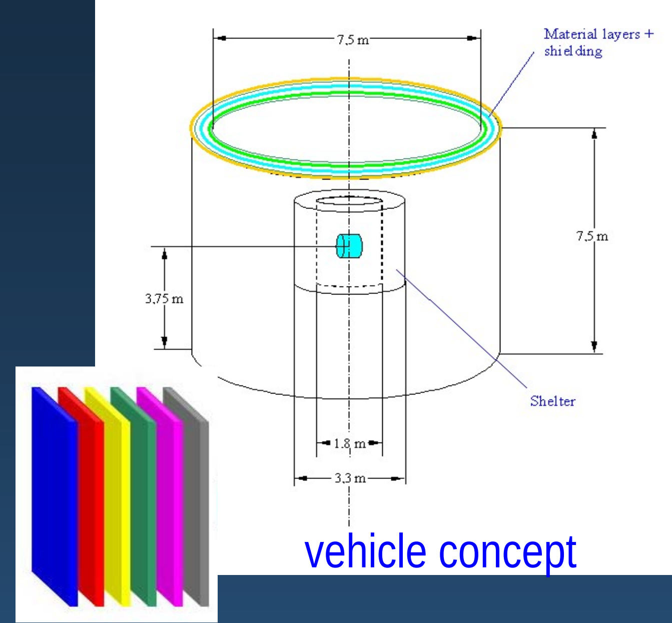
	p-value		
	CvM	KS	AD
Left branch	0.977		
Right branch		0.985	
Whole curve			0.994



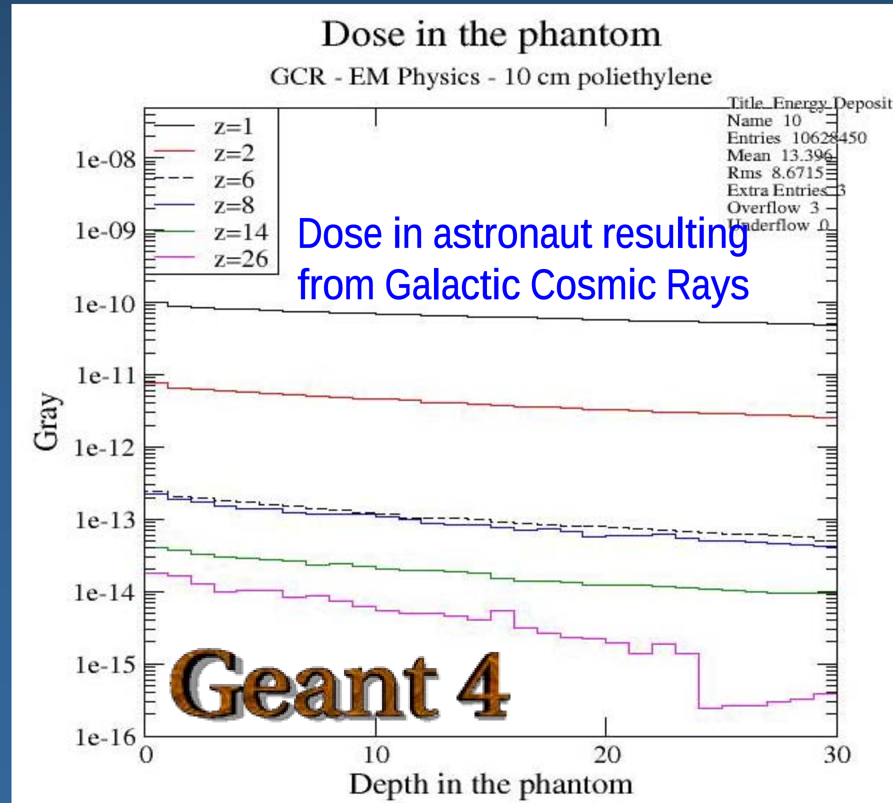


GEANT4 simulation

Dosimetry in interplanetary missions



vehicle concept



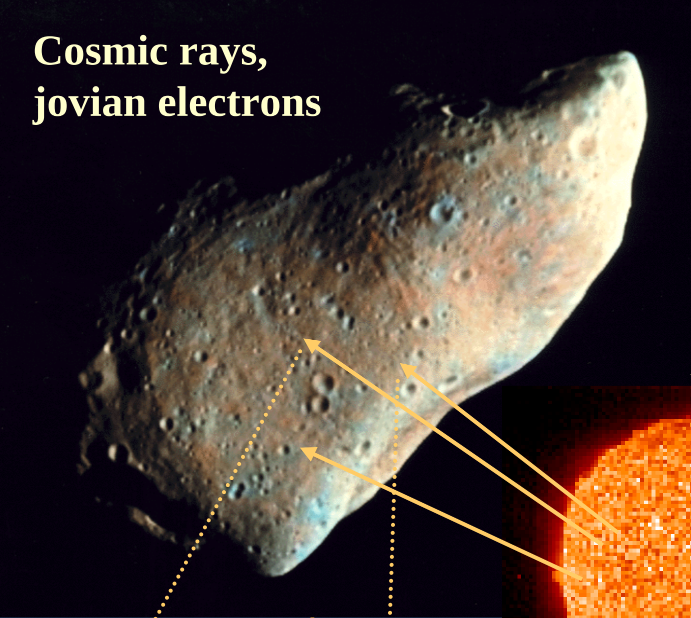
Dose in astronaut resulting from Galactic Cosmic Rays

Alenia SPAZIO UNA SOCIETA' FINMECCANICA EADS RxTec

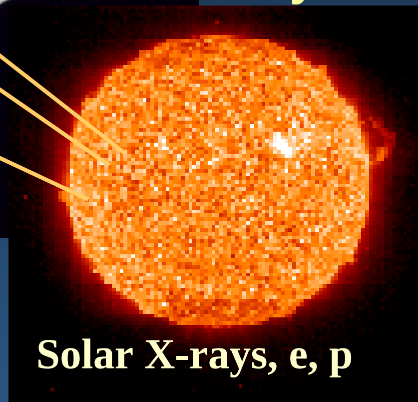
Maria Grazia Pia, *INFN Genova*

Solar system explorations

Study of the elemental composition of planets, asteroids and moons ⟶ clues to solar system formation



Courtesy SOHO EIT

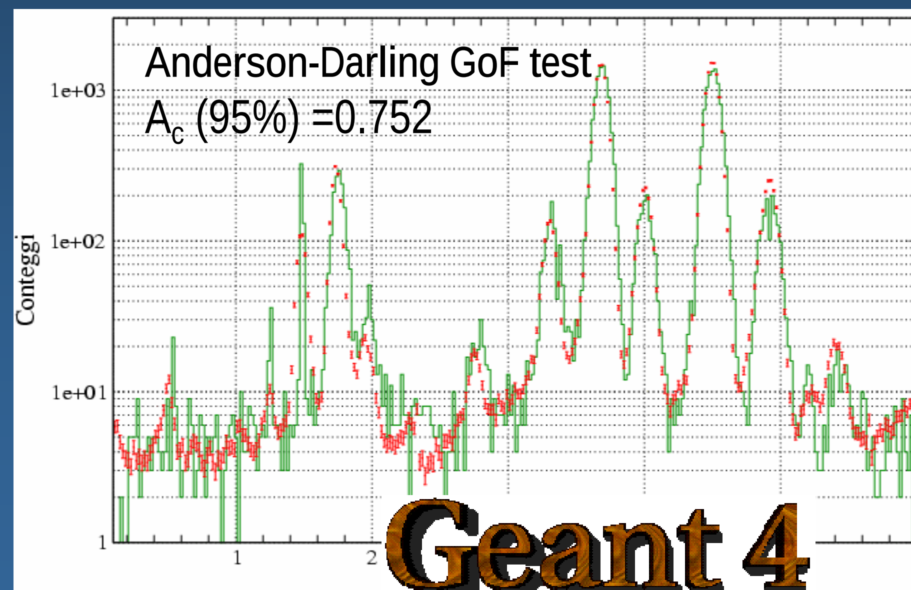


X-ray fluorescence Arising from the solar X-ray flux, sufficient, for the inner planets, to significant fluorescence fluxes to an orbiter

PIXE Significant only during particle events, during which it can exceed XRF

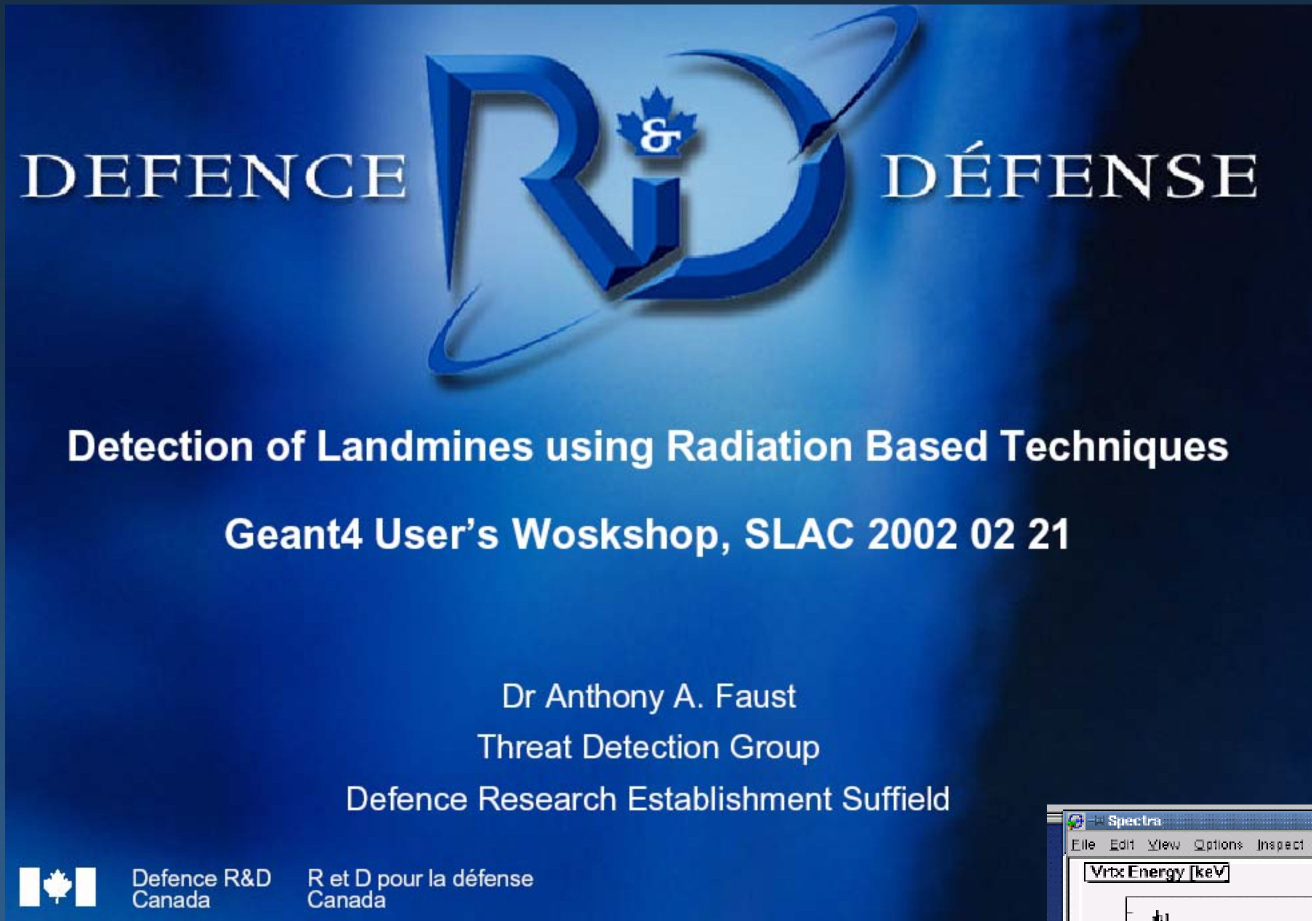
BepiColombo
ESA cornerstone mission to Mercury

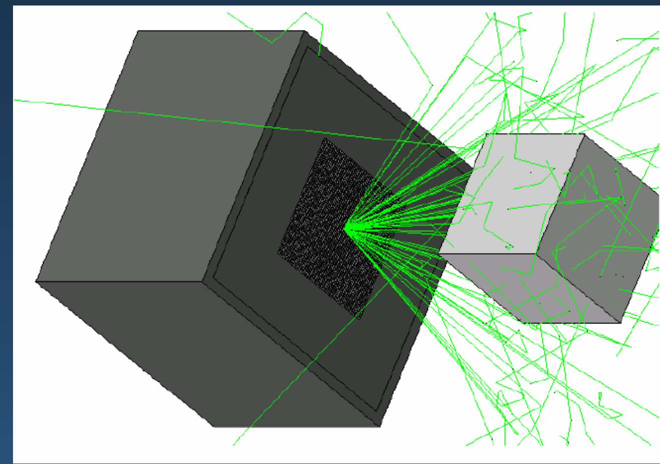
Courtesy of ESA Astrophysics

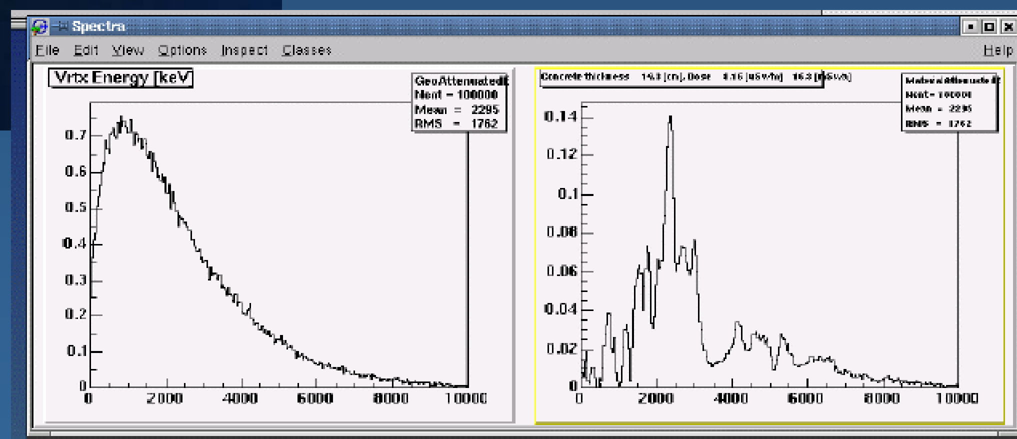


Fluorescence spectrum from Hawaiian basalt: experimental data and simulation

Maria







X-ray Backscatter Imaging

- Exploit Z dependent differences in Compton/Photoelectric cross-sections
- $Z^{mine}_{eff} \sim 8$ and $Z^{soil}_{eff} \sim 14$

Used Low Energy packages

Polarisation

Cross section:

$$\frac{d\sigma}{d\Omega} = \frac{1}{2} r_0^2 \frac{h\nu^2}{h\nu_0^2}\left[\frac{h\nu_0}{h\nu} + \frac{h\nu}{h\nu_0} - 2\sin^2\theta\cos^2\phi\right]$$

Low Energy Polarised Compton

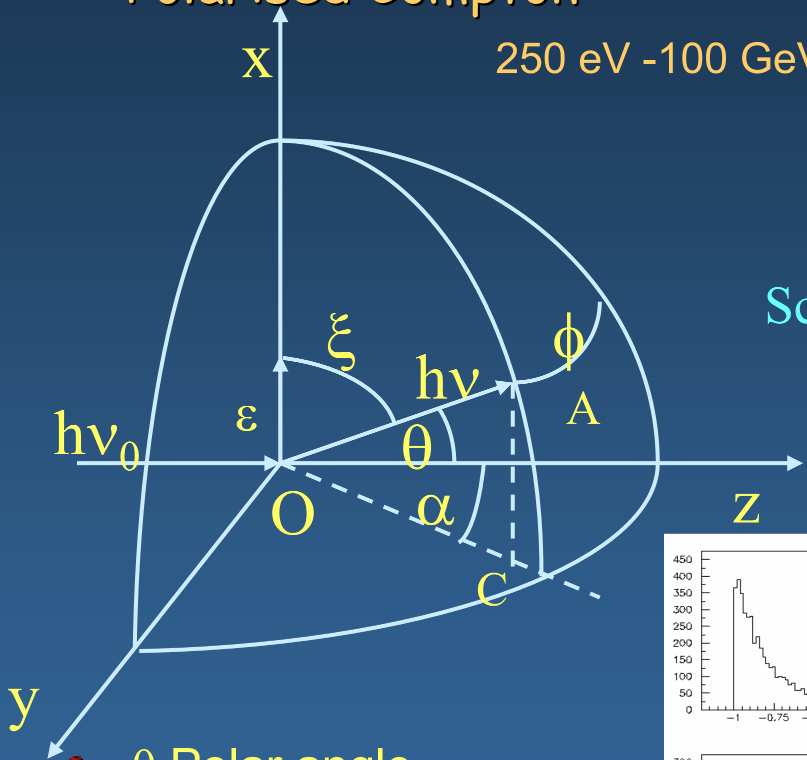
250 eV -100 GeV

Sample Methods:

Integrating over ϕ

- Sample θ
- θ - Energy Relation $\Rightarrow$ Energy
- Sample of ϕ from $P(\phi) = a\,(b - c\cos^2\phi)$ distribution

$$\cos\xi = \sin\theta\cos\phi \quad \Rightarrow \quad \sin\xi = \sqrt{1-\sin^2\theta\cos^2\phi} = N$$

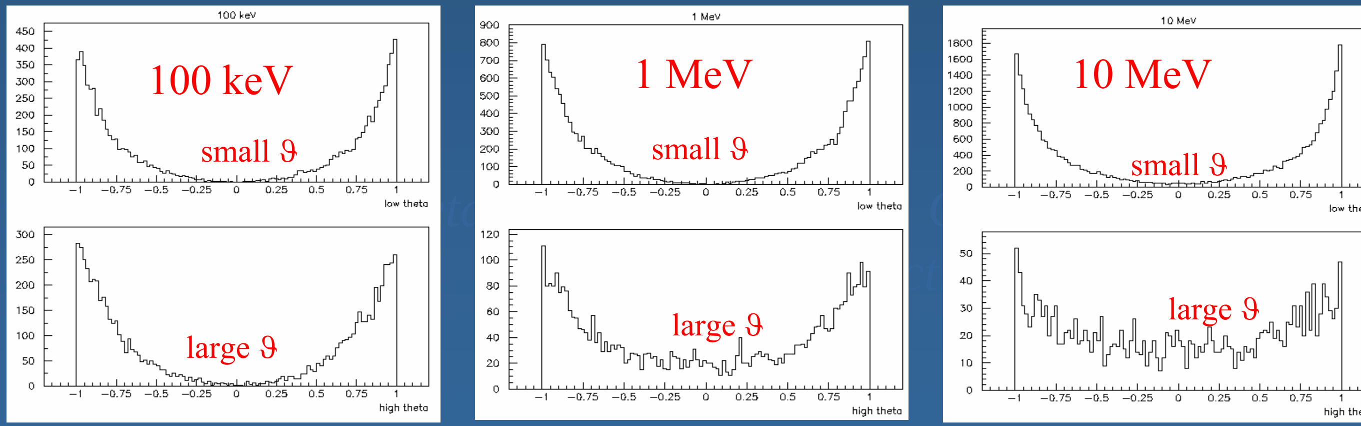


Scattered Photon Polarization

$$\overline{\varepsilon'_{\perp}} = \frac{1}{N}\left(\cos\theta\,\hat{j} - \sin\theta\sin\phi\,\hat{k}\right)\sin\beta$$

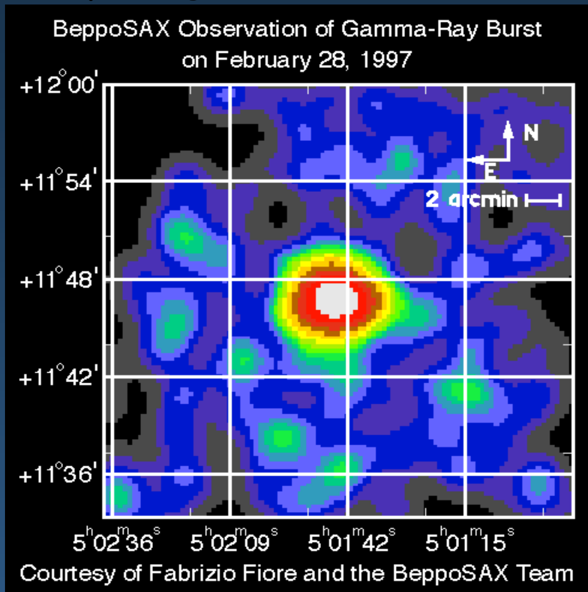
$$\overline{\varepsilon'_{\parallel}} = \left(N\hat{i} - \frac{1}{N}\sin^2\theta\,\sin\phi\,\cos\phi\,\hat{j} - \frac{1}{N}\sin\theta\,\cos\theta\,\cos\phi\,\hat{k}\right)\cos\beta$$

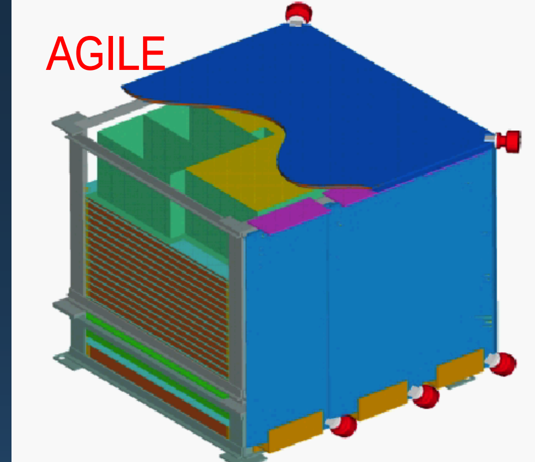
- θ Polar angle
- ϕ Azimuthal angle
- ε Polarization vector

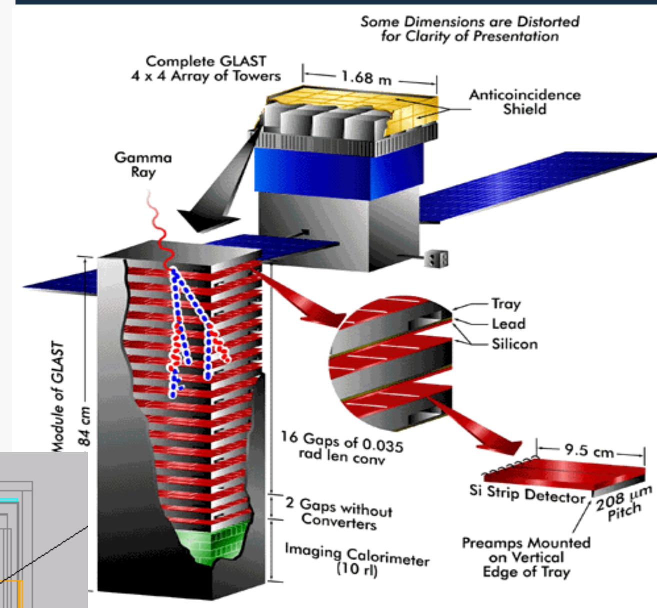


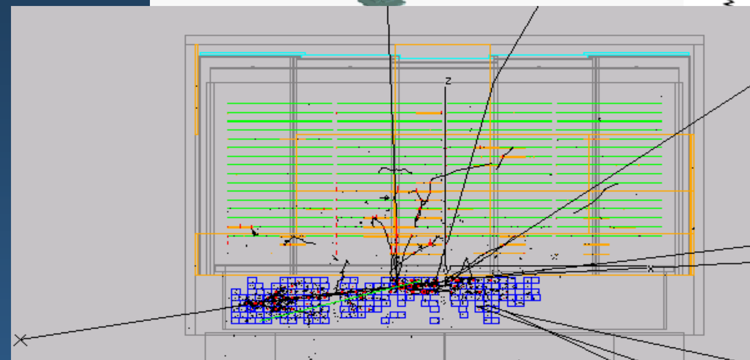
γ astrophysics

γ-ray bursts

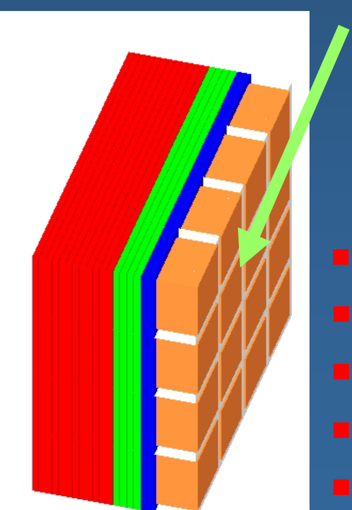








GLAST



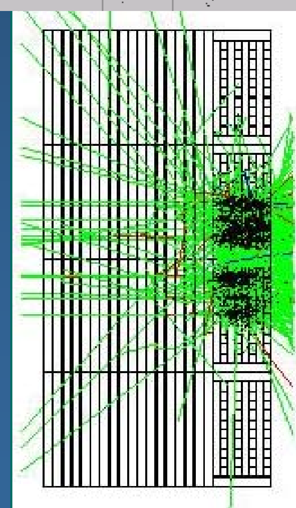
Typical telescope:

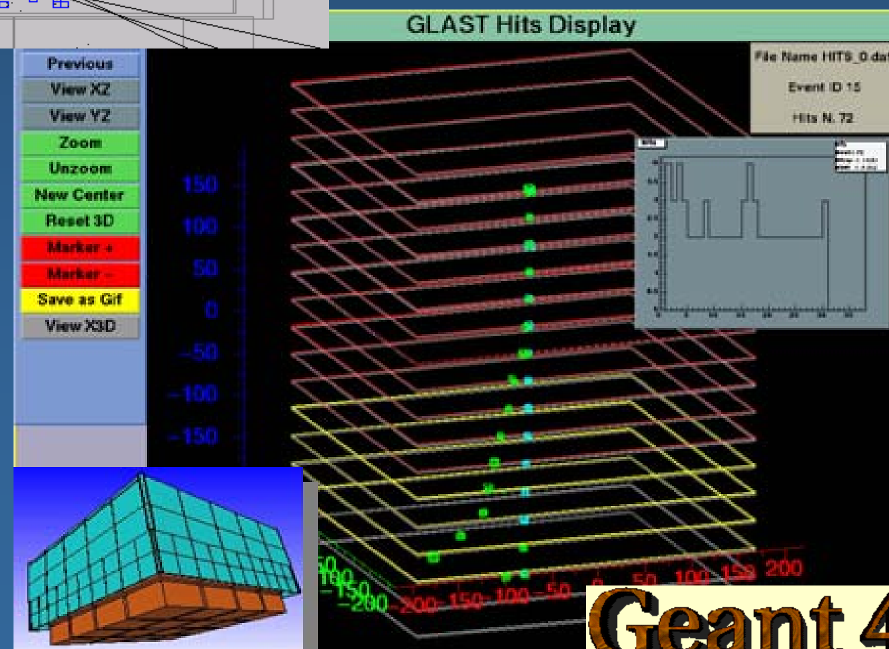
Tracker

Calorimeter

Anticoincidence

- γ conversion
- electron interactions
- multiple scattering
- δ-ray production
- charged particle tracking

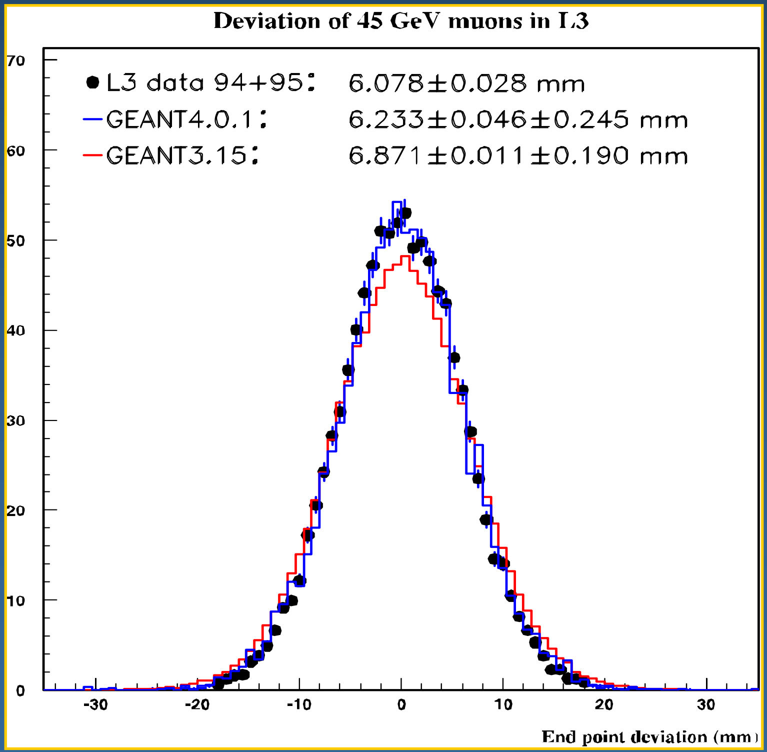




Geant 4

Muons

- 1 keV up to 10 PeV scale
- simulation of ultra-high energy and cosmic ray physics
- High energy extensions based on theoretical models



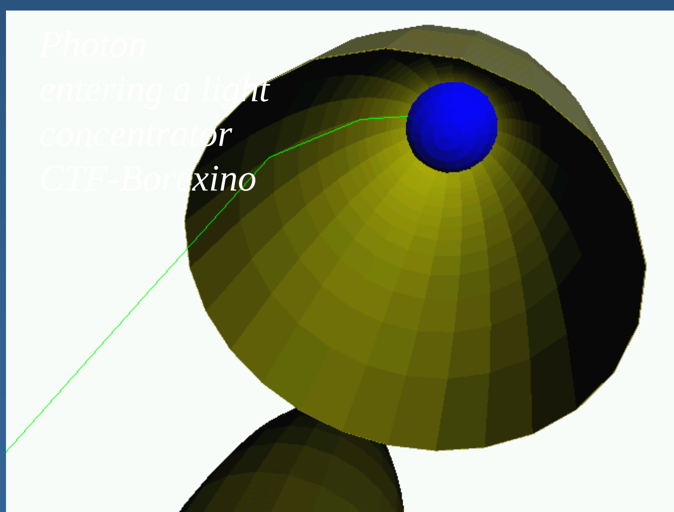
- Muon Muon energy loss
- Muon radiation processes
- Gamma conversion to muon pair
- Positron annihilation to muon pair
- Positron annihilation into hadrons

Optical photons

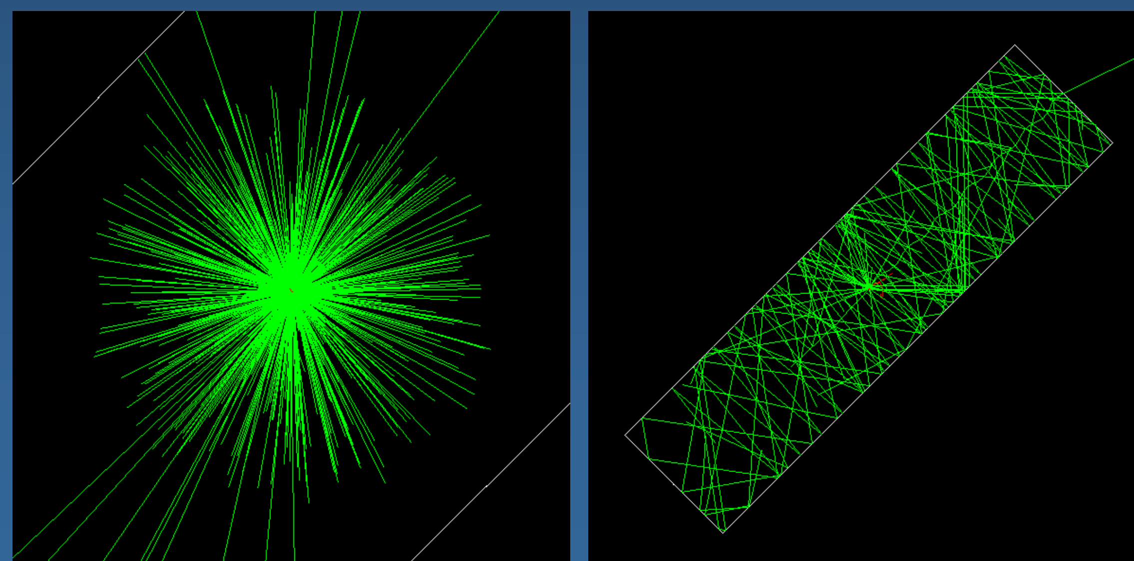
Production of optical photons in HEP detectors is mainly due to Cherenkov effect and scintillation

Processes in Geant4:

- in-flight absorption
- Rayleigh scattering
- medium-boundary interactions (reflection, refraction)



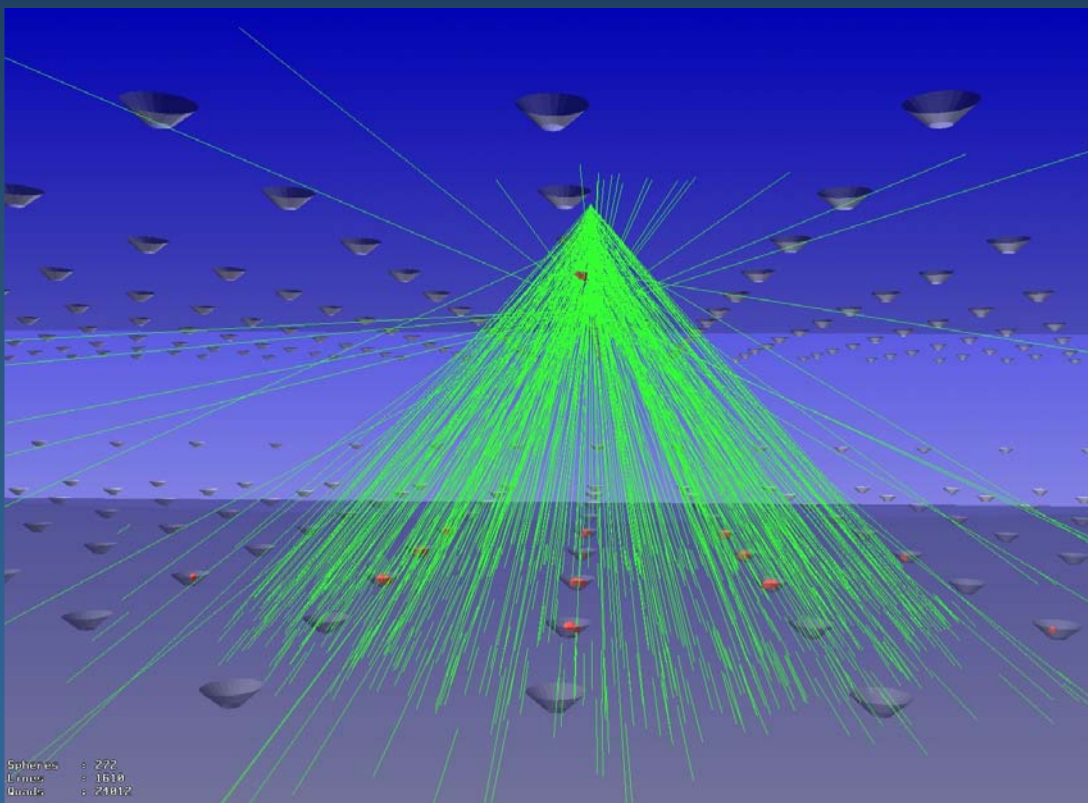
Geant4 Optical Processes : Scintillating Cells and WLS Fibers

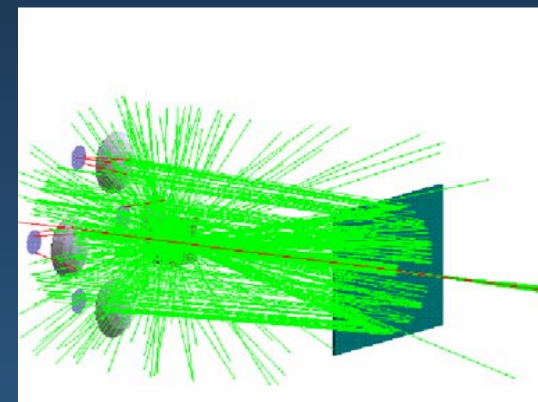


Courtesy of J. Mc Cormick (SLAC)

Cherenkov

Milagro is a Water-Cherenkov detector located in a 60m x 80m x 8m covered pond near Los Alamos, NM



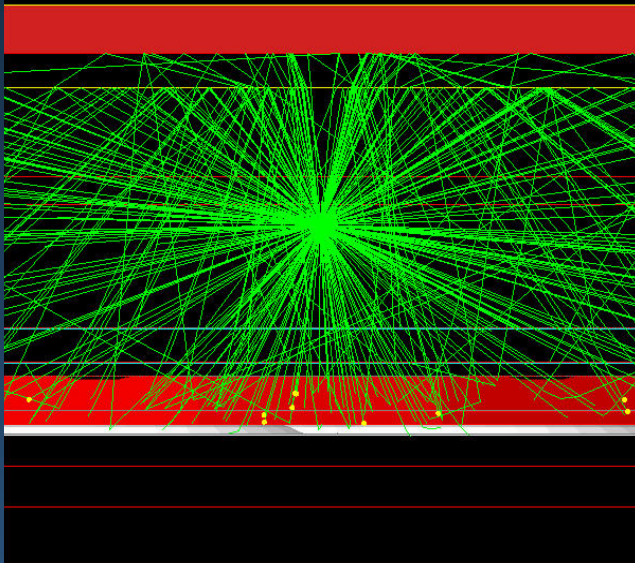


LHCb

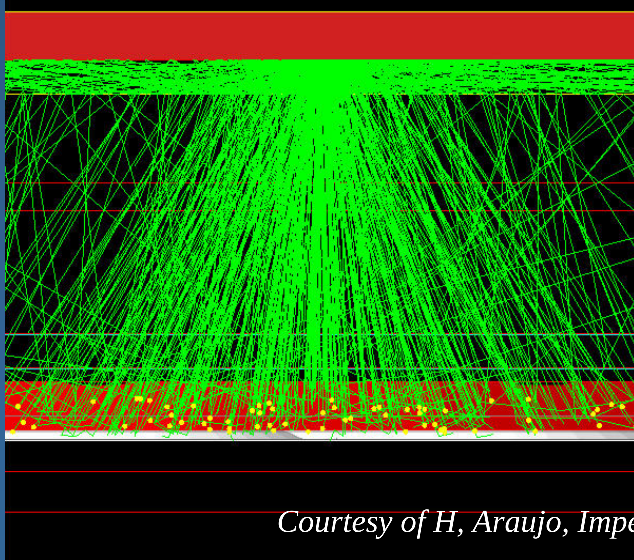
Aerogel Thickness		Yield Per Event	Cherenkov Angle mrad
4 cm	DATA	6.3 ± 0.7	247.1+-5.0
	MC	7.4 ± 0.8	246.8+-3.1
8 cm	DATA	9.4 ± 1.0	245.4+-4.8
	MC	10.1 ±1.1	243.7+-3.0

Scintillation

prompt scintillation

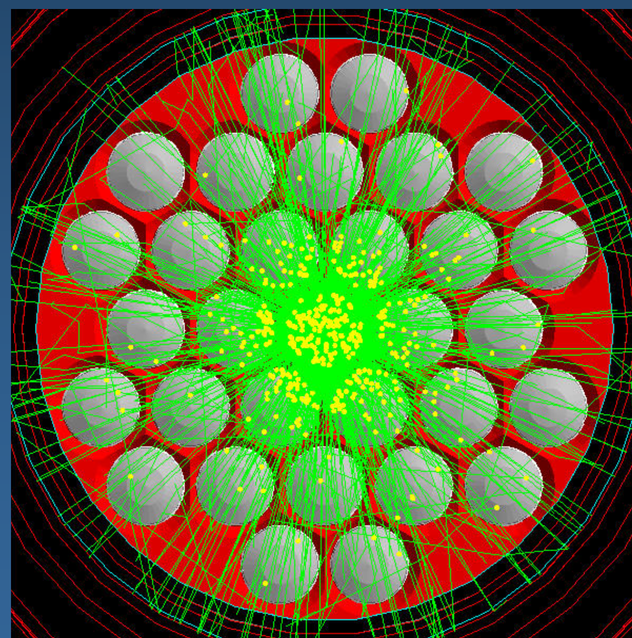


termoluminescense

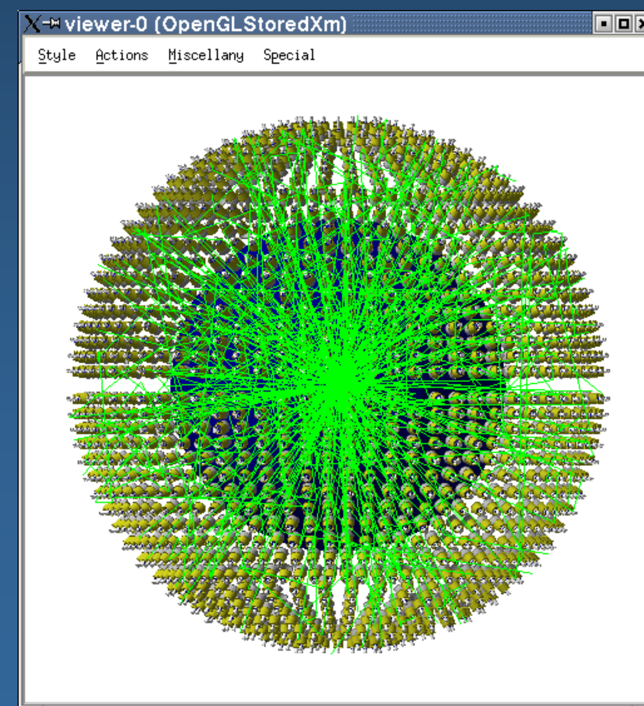


ZEPLIN III
Dark Matter Detector

signal in PMT



GEANT4 Scintillation
Event in BOREXINO



Courtesy of H, Araujo, Imperial College London

Hadronic physics

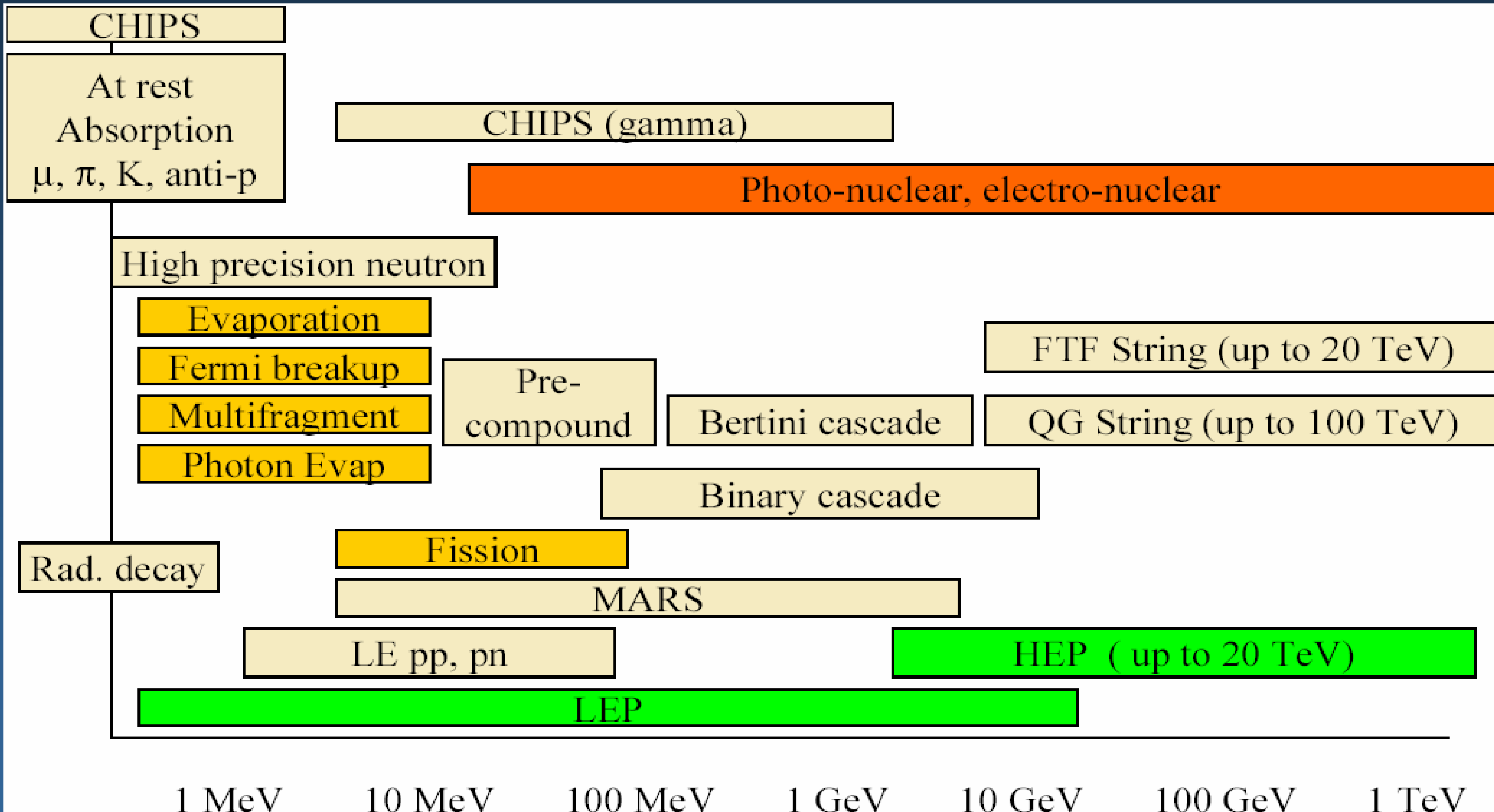
- Completely different approach w.r.t. the past (Geant3)
  - native
  - transparent
  - no longer interface to external packages
  - clear separation between data and their use in algorithms

- Cross section data sets
  - transparent and interchangeable

- Final state calculation
  - models by particle, energy, material

- Ample variety of models
  - the most complete hadronic simulation kit on the market
  - alternative and complementary models
  - data-driven, parameterised and theoretical models

Hadronic model inventory

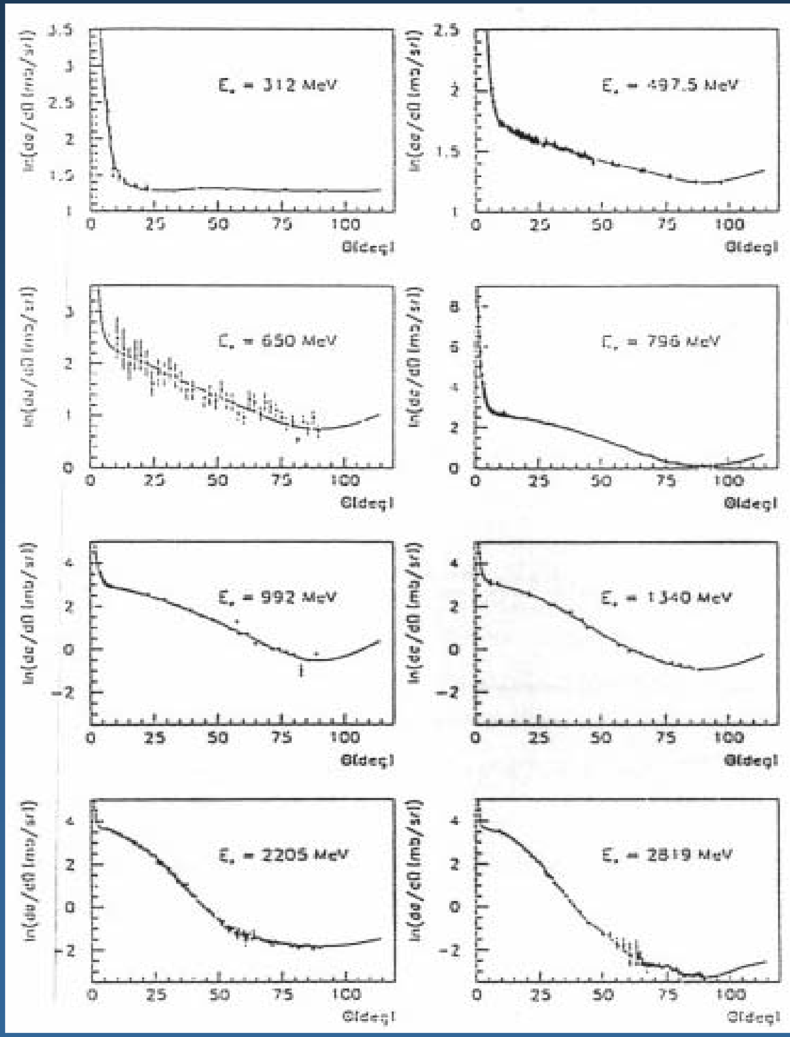


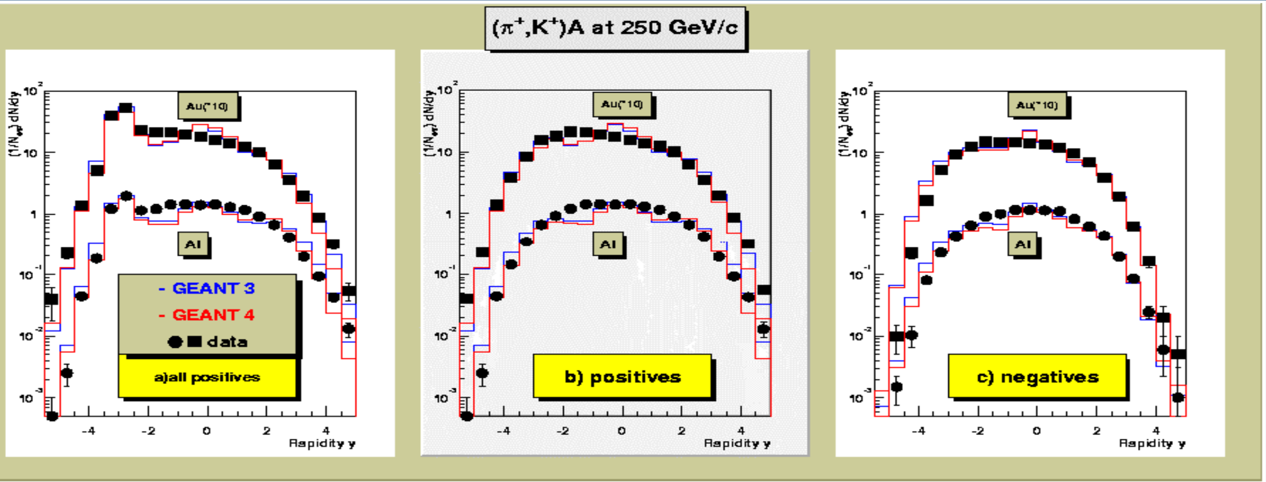
Parameterised and data-driven hadronic models (1)

Based on experimental data

- Some models originally from GHEISHA
  - completely reengineered into OO design
  - refined physics parameterisations
- New parameterisations
  - pp, elastic differential cross section
  - nN, total cross section
  - pN, total cross section
  - np, elastic differential cross section
  - πN, total cross section
  - πN, coherent elastic scattering

p elastic scattering on Hydrogen

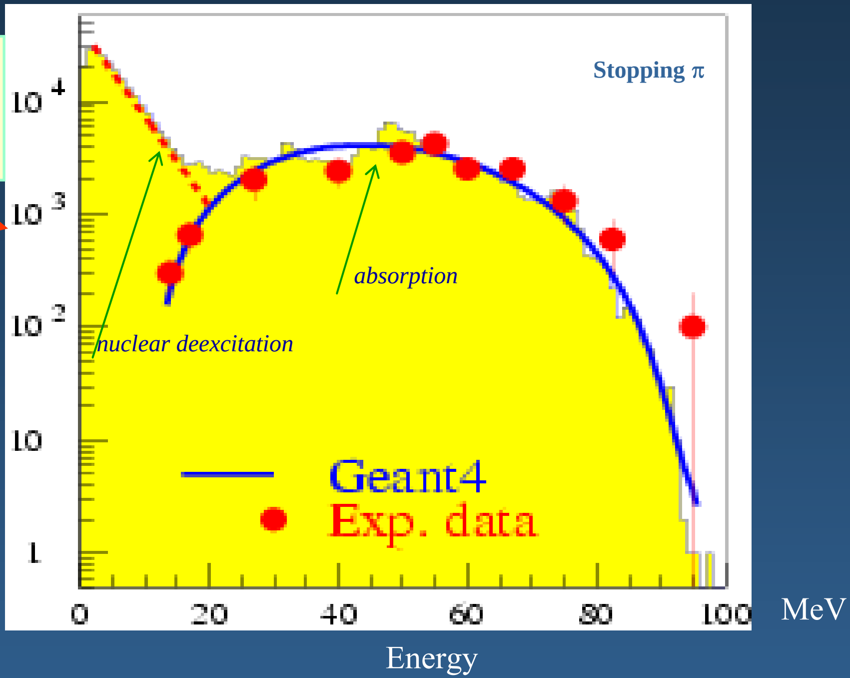


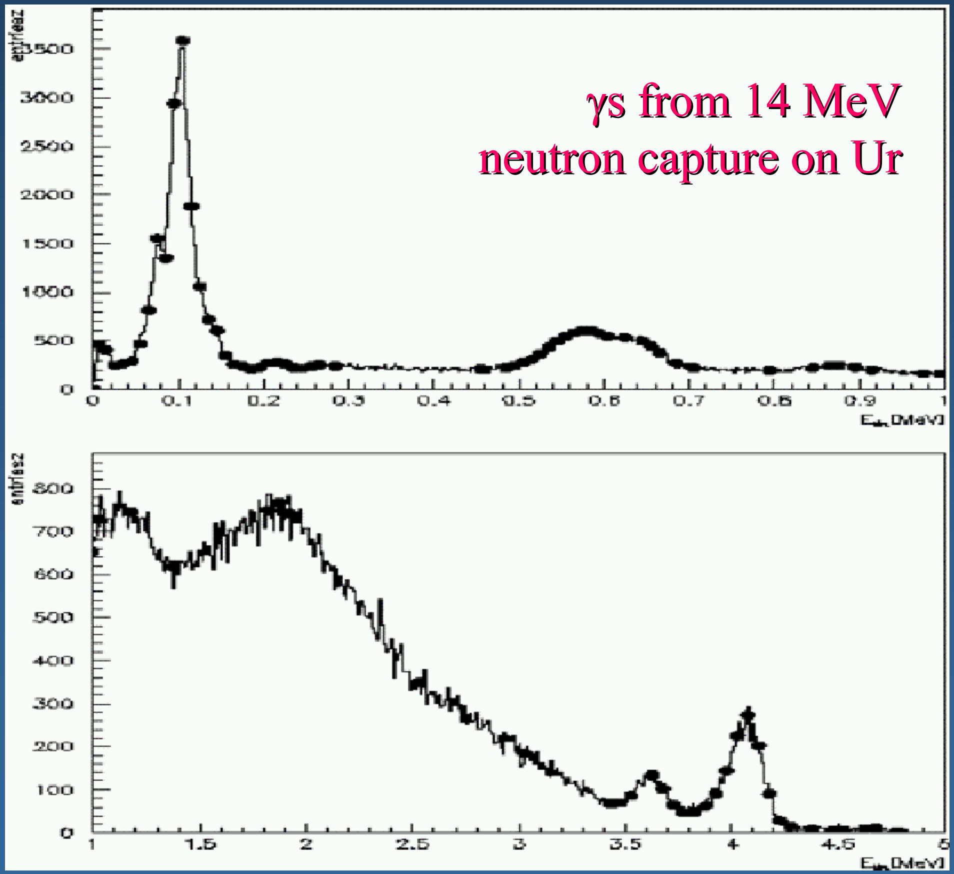


Parameterised and data-driven hadronic models (2)

Other models are completely new, such as:

stopping particles: π^-, K^-
(relevant for μ/π PID detectors)





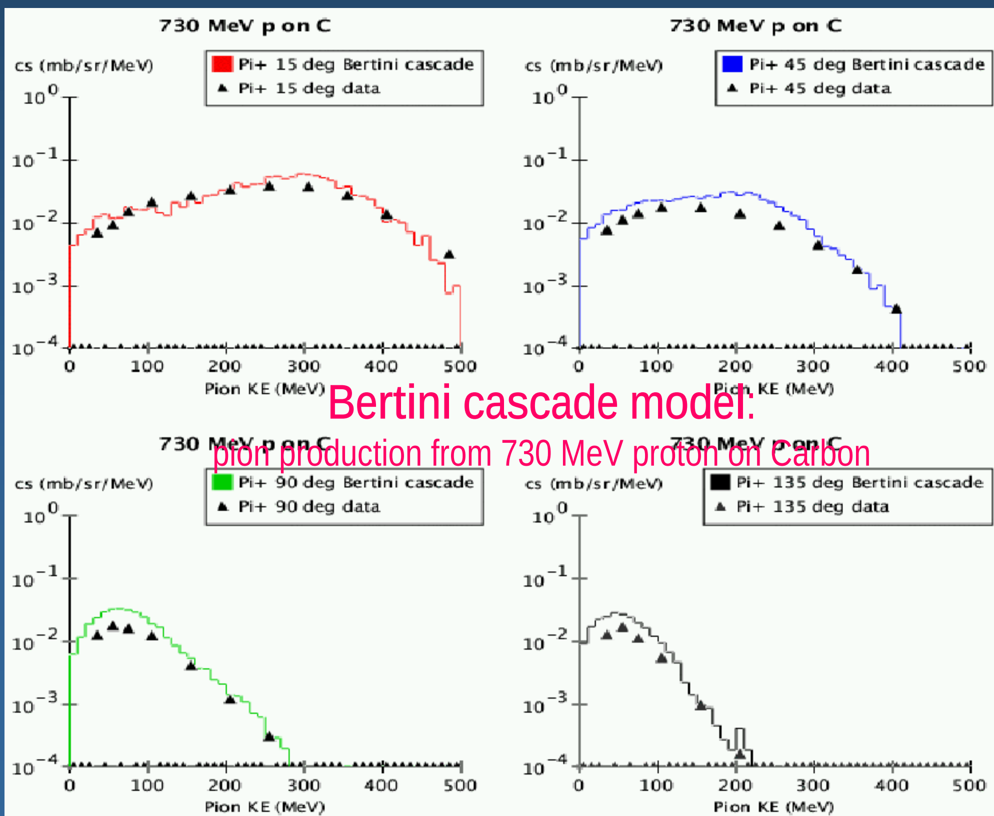
neutrons

<u>All</u> worldwide existing databases used in **neutron** transport

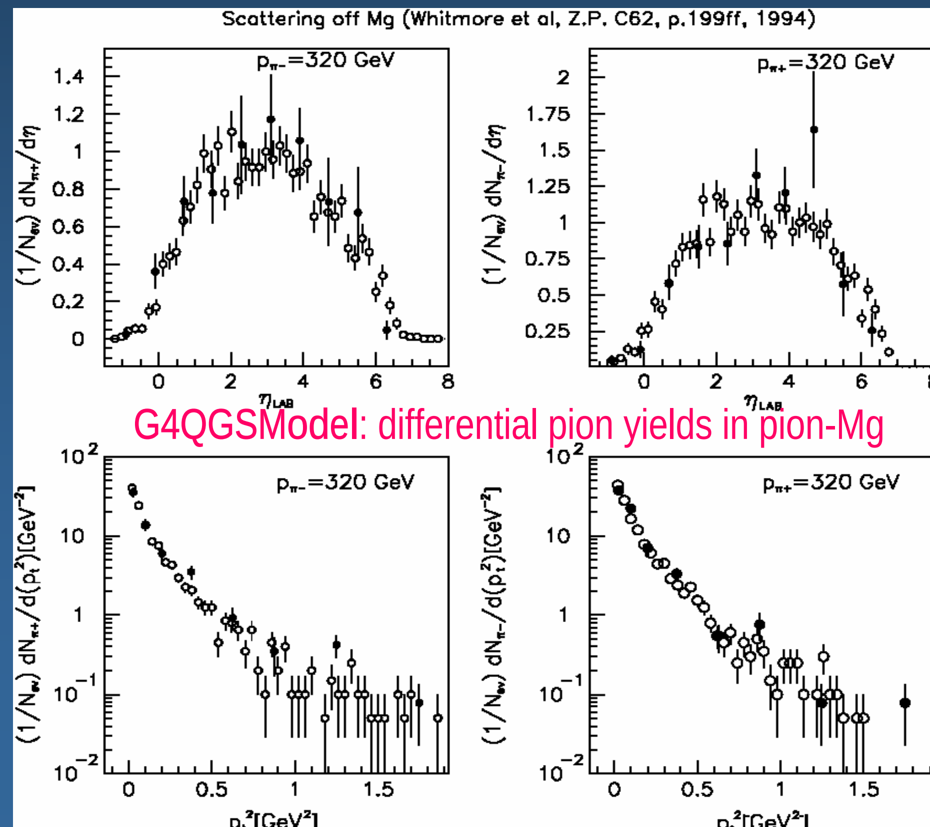
Brond, CENDL, EFF, ENDFB, JEF, JENDL, MENDL etc.

Theory-driven models

- Complementary and alternative models
- *Evaporation phase*
- Low energy range O(100 MeV)**:** *pre-equilibrium*
- Intermediate energy range, O(100 MeV) to O(5 GeV): *intra-nuclear transport*
- High energy range: *hadronic generator* régime

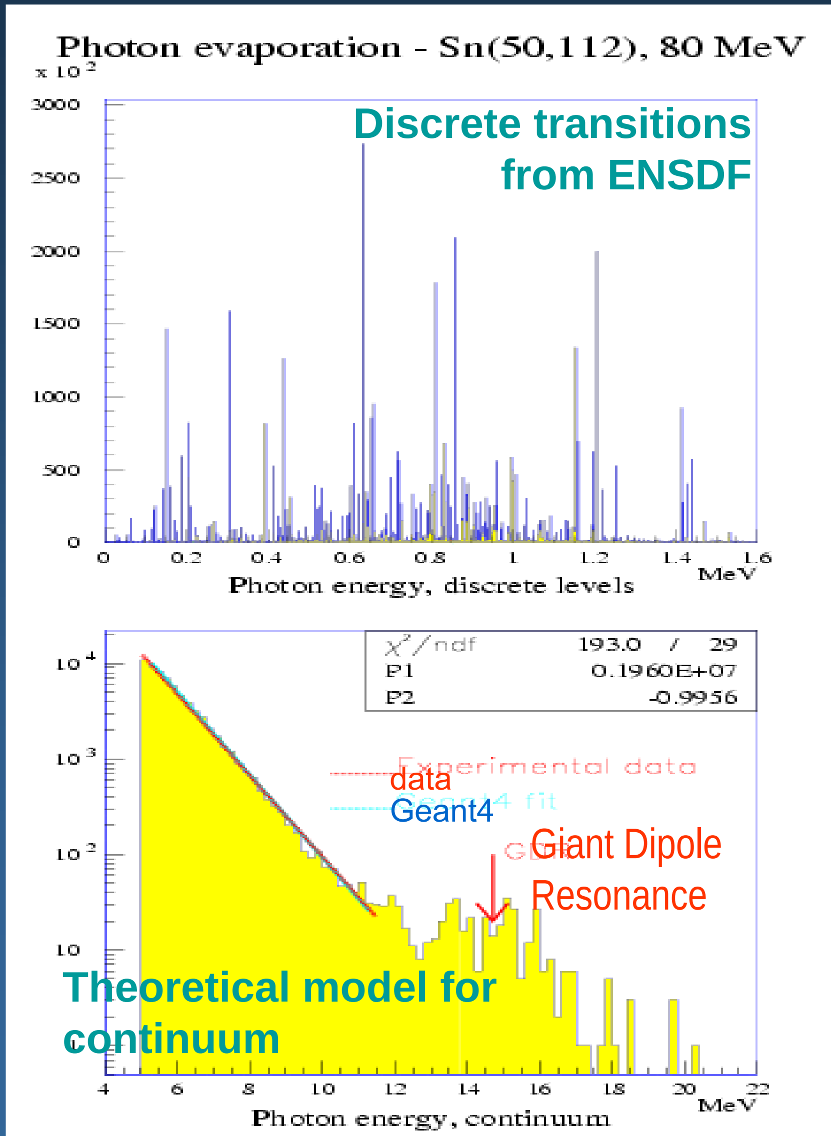


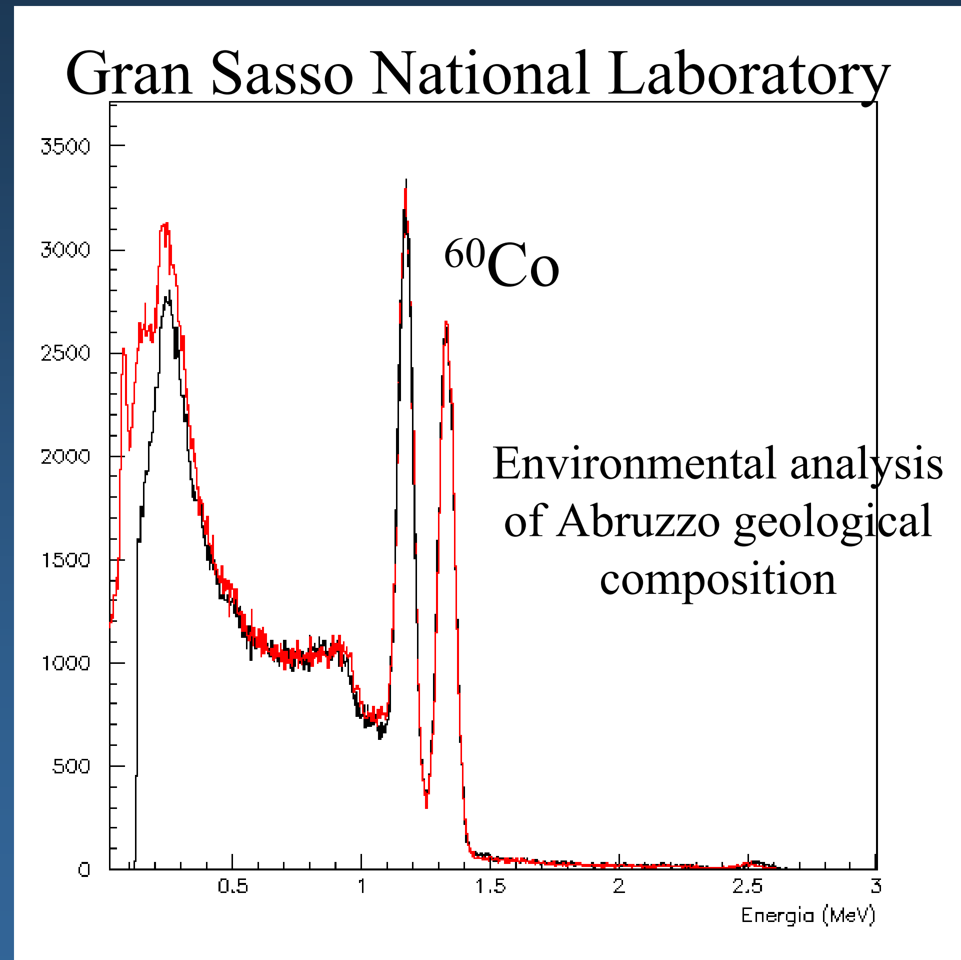
Bertini cascade model:
pion production from 730 MeV proton on Carbon



G4QGSModel: differential pion yields in pion-Mg

The two worlds can be mixed…





Other components

- Materials
  – elements, isotopes, compounds, chemical formulae
- Particles
  – all PDG data
  – and more, for specific Geant4 use, like ions
- Hits & Digi
  – to describe detector response
- Primary event generation
  – some general purpose tools provided within the Toolkit
    - eg. GeneralParticleSource
- ...and much more (no time to mention all!)

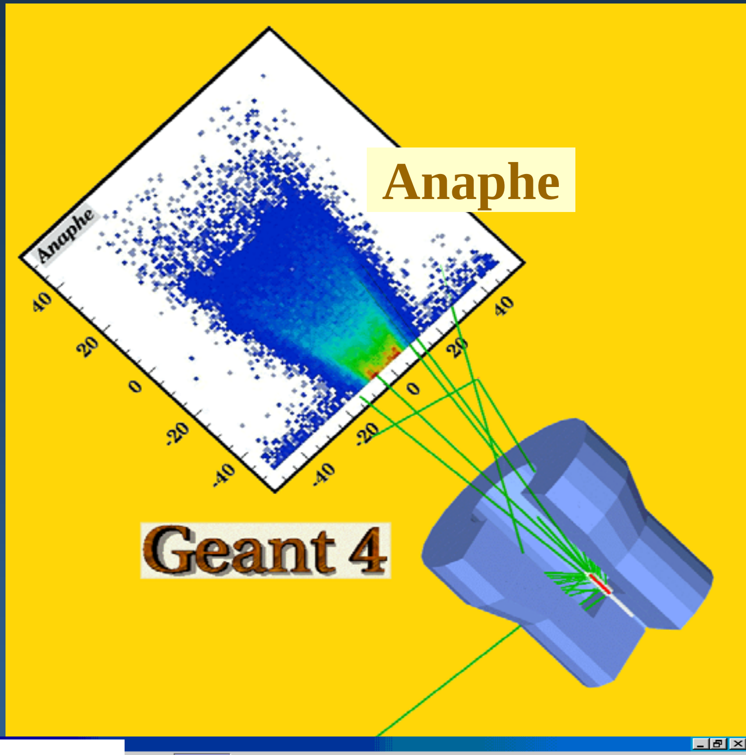
read-out geometry
event biasing
fast simulation
parallelisation
persistency
much more physics
etc.

Interface to external tools in Geant4

Through *abstract interfaces*

no dependence

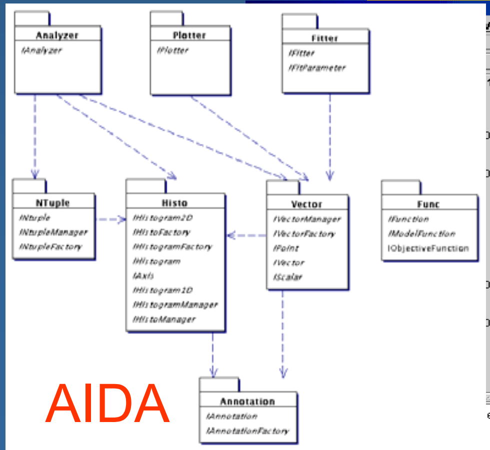
minimize coupling of components

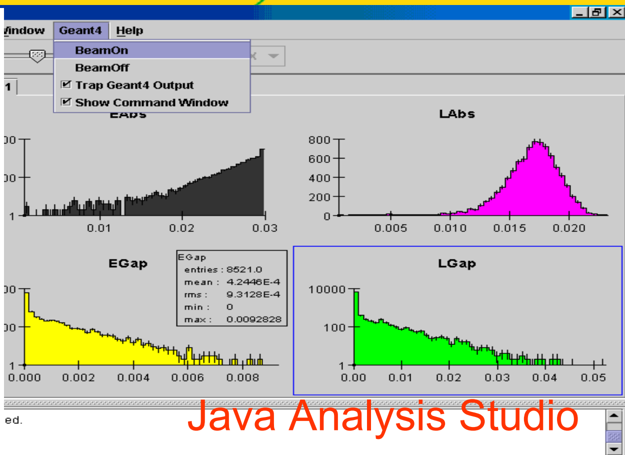


Similar approach

- Visualisation
- (G)UI
- Persistency
- Analysis

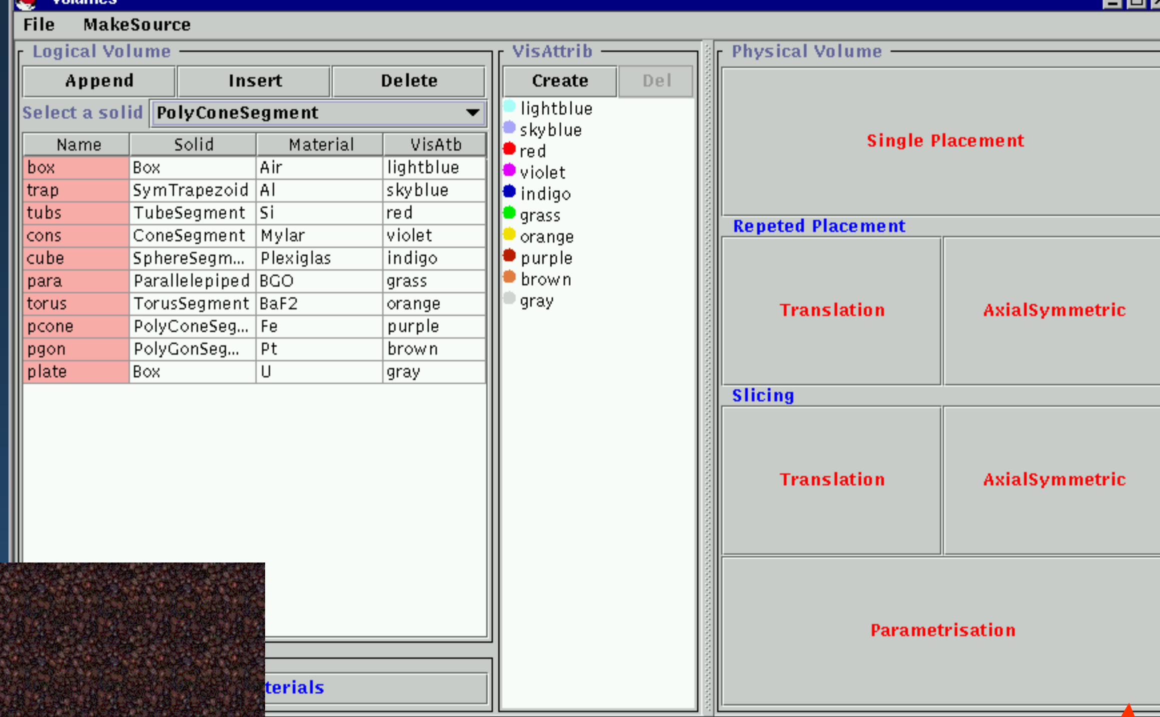
The user is free to choose the concrete system he/she prefers for each component

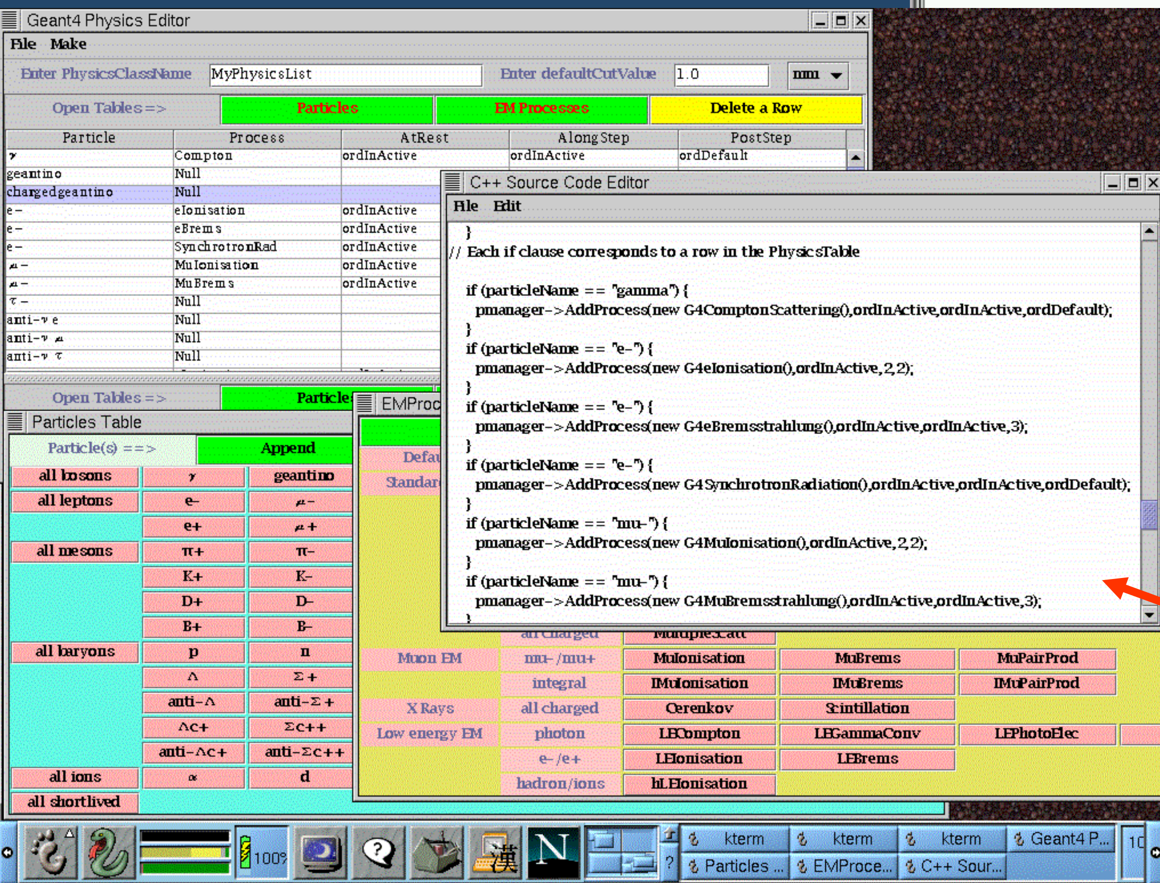




User Interface

- Several implementations, all handled through abstract interfaces
- Command-line (batch and terminal)
- GUIs
  - X11/Motif, GAG, MOMO, OPACS, Java

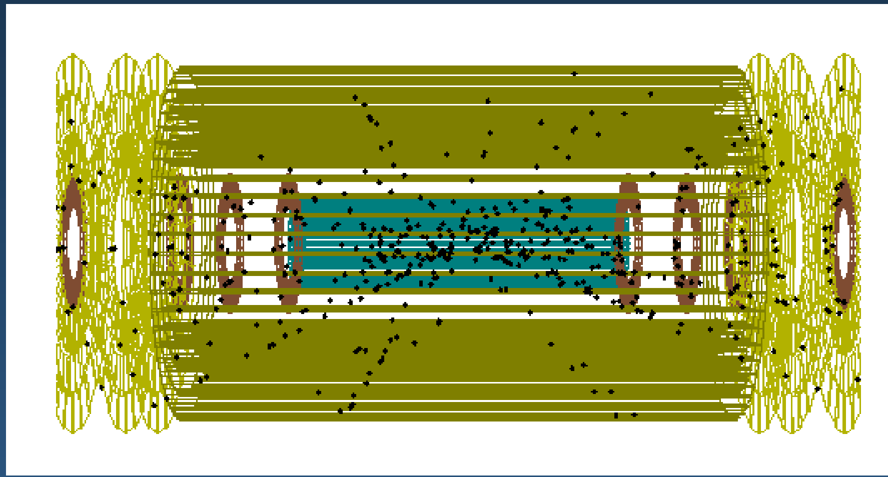


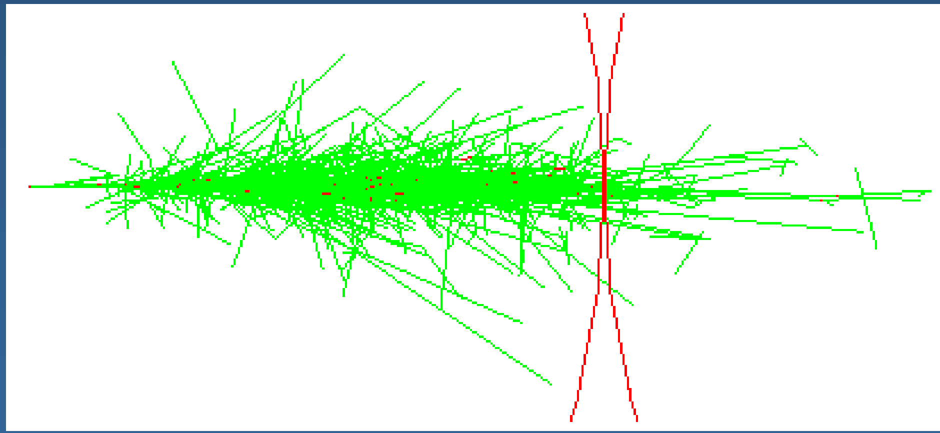


- Automatic code generation for geometry and physics through a GUI
  - GGE (Geant4 Geometry Editor)
  - GPE (Geant4 Physics Editor)

Visualisation

- Control of several kinds of visualisation
  - detector geometry
  - particle trajectories
  - hits in the detectors
- Various drivers
  - OpenGL
  - OpenInventor
  - X11
  - Postscript
  - DAWN
  - OPACS
  - HepRep
  - VRML…
- all handled through abstract interfaces

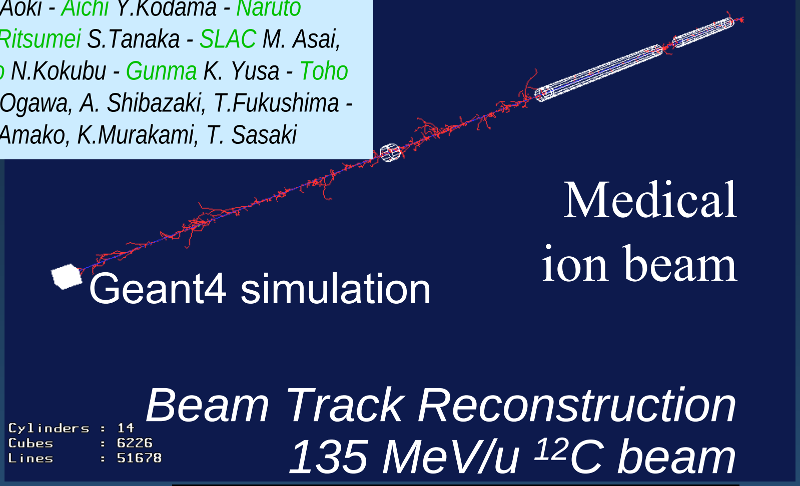


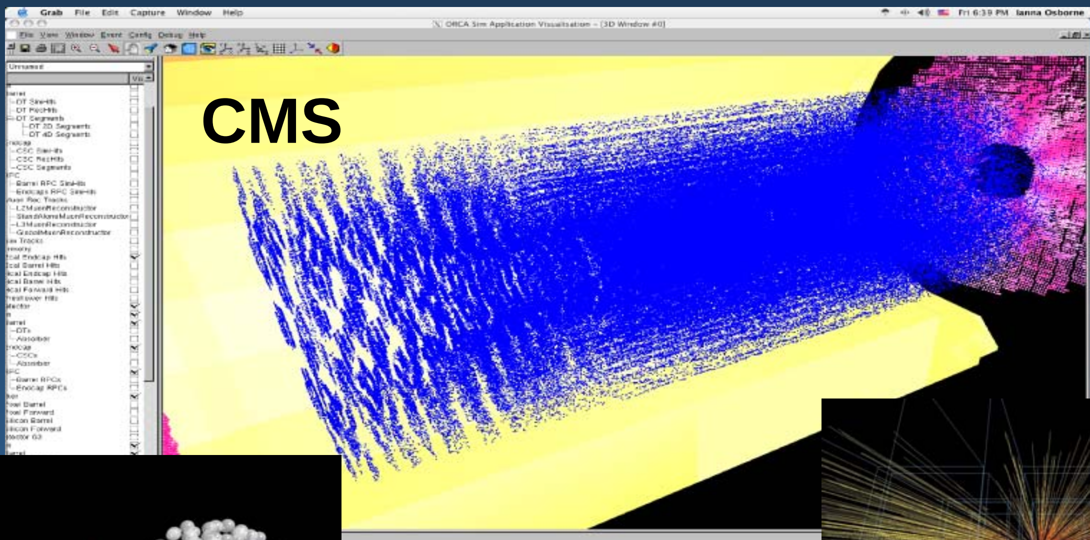


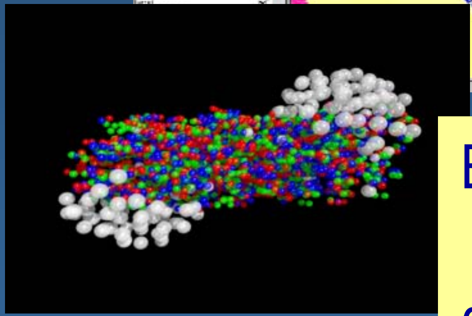
Pushing Geant4 to the limit

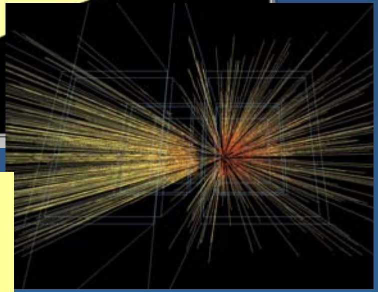
Heavy ion beams

NIRS N. Kanematsu, M. Komori - Nagoya K. Niwa, T.Toshito, T.Nakamura, T.Ban, N.Naganawa, S.Takahashi - Uchu-ken M.Ozaki - Kobe S. Aoki - Aichi Y.Kodama - Naruto H.Yoshida - Ritsumei S.Tanaka - SLAC M. Asai, T. Koi - Tokyo N.Kokubu - Gunma K. Yusa - Toho H.Shibuya, R.Ogawa, A. Shibazaki, T.Fukushima - KEK K. Amako, K.Murakami, T. Sasaki

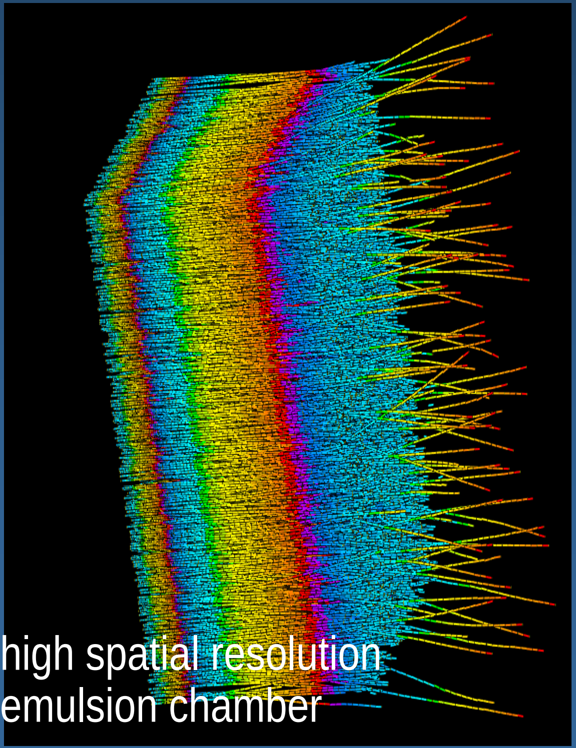








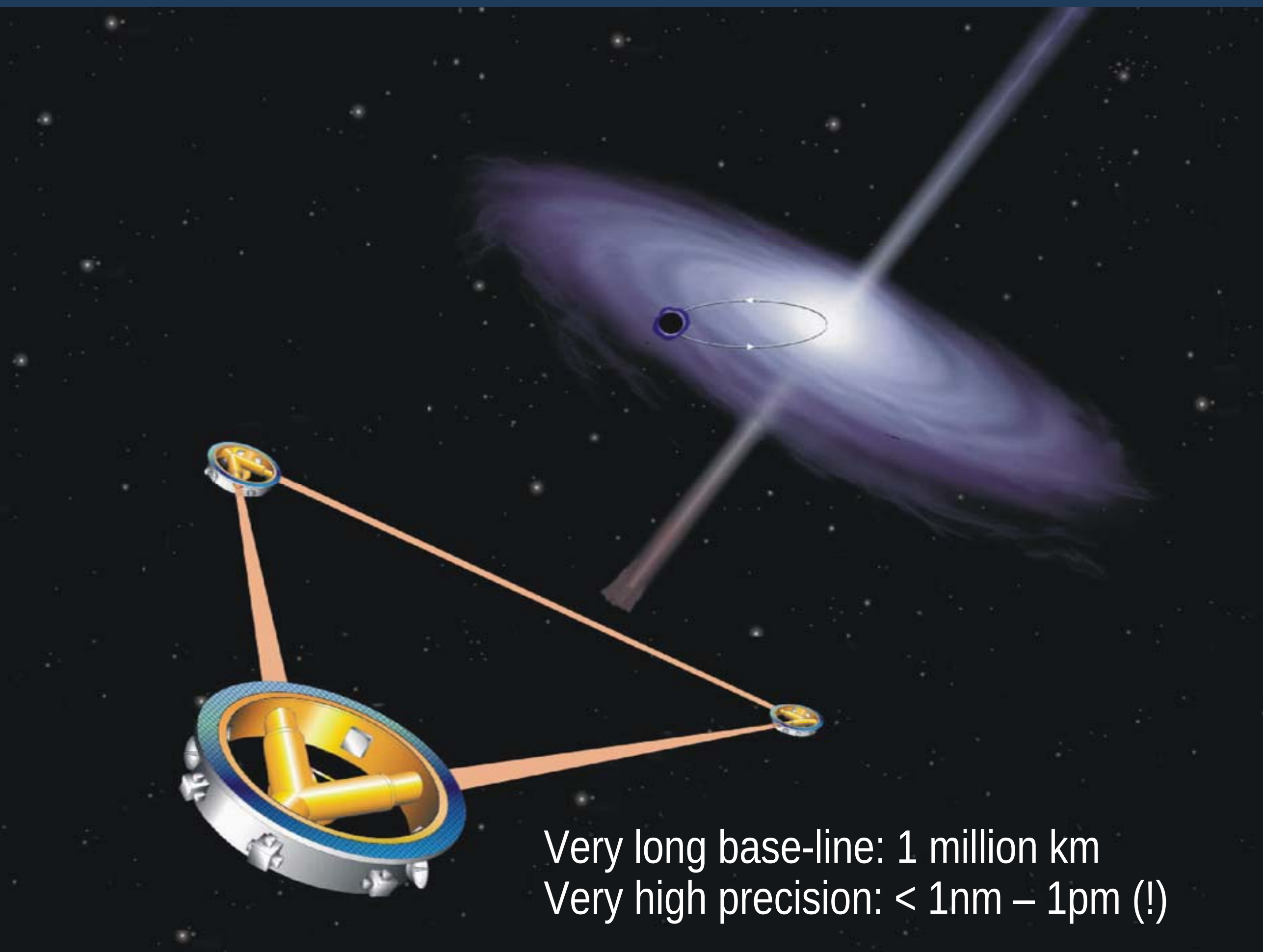
Events with > 50000 particles/event in detector acceptance

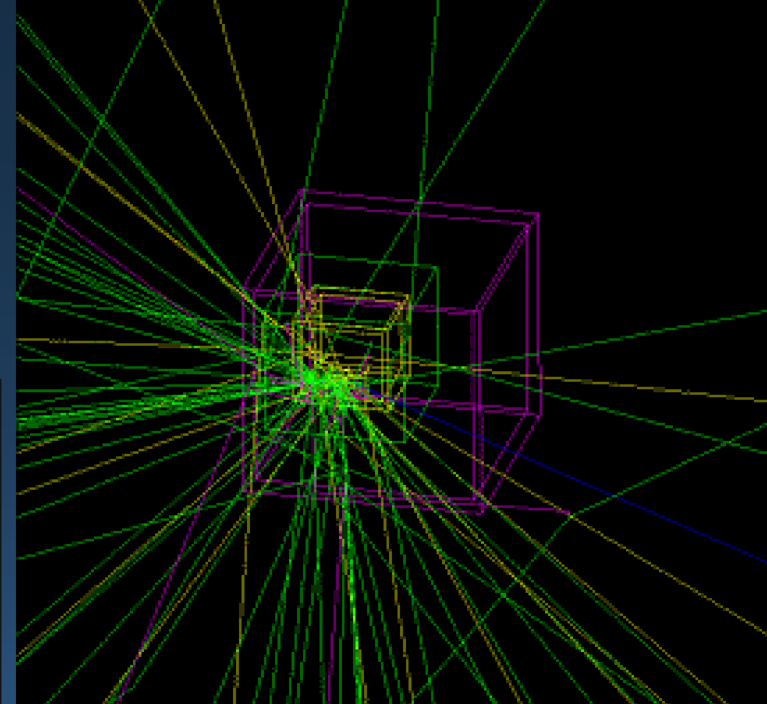


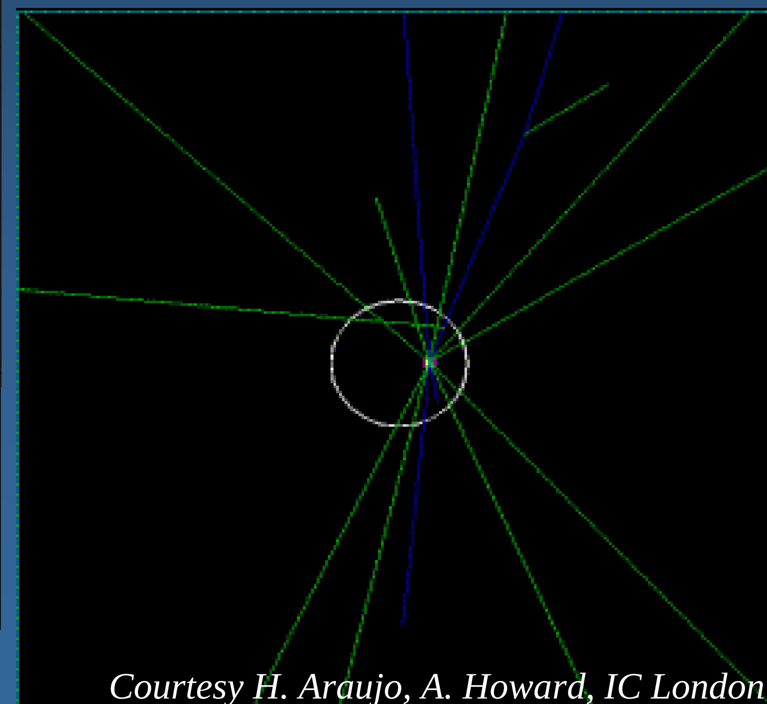
~ 180 minutes to simulate 1 event with 55K generator tracks

LISA (gravitational waves)

Geant4 relevant for evaluation of space charging effects







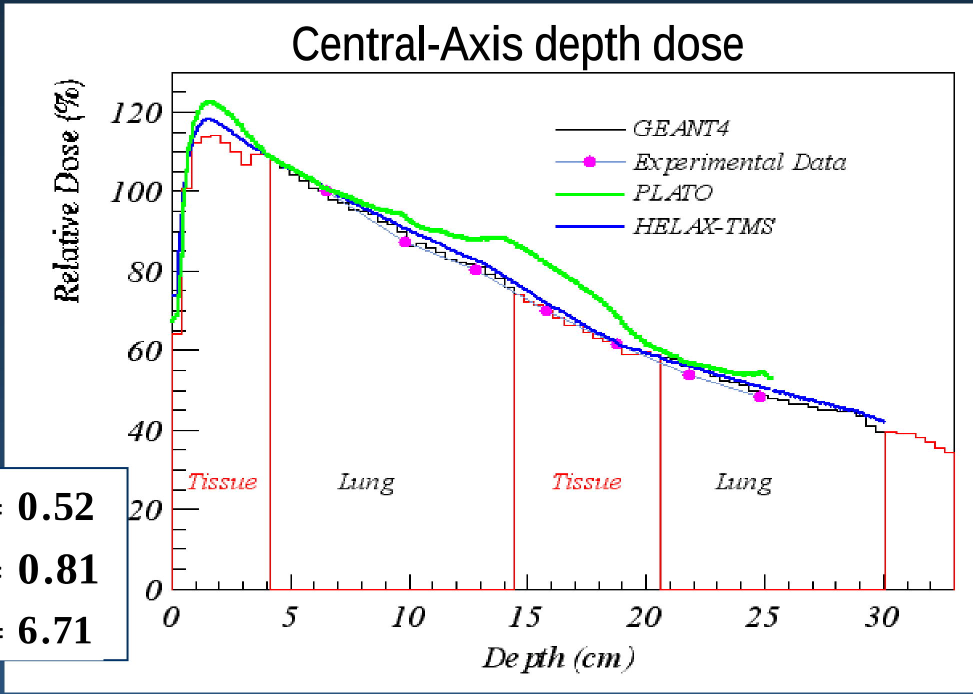
Courtesy H. Araujo, A. Howard, IC London

Is it worthwhile?

Comparison with commercial radiotherapy treatment planning systems

M. C. Lopes
IPOFG-CROC Coimbra Oncological Regional Center
L. Peralta, P. Rodrigues, A. Trindade
LIP - Lisbon

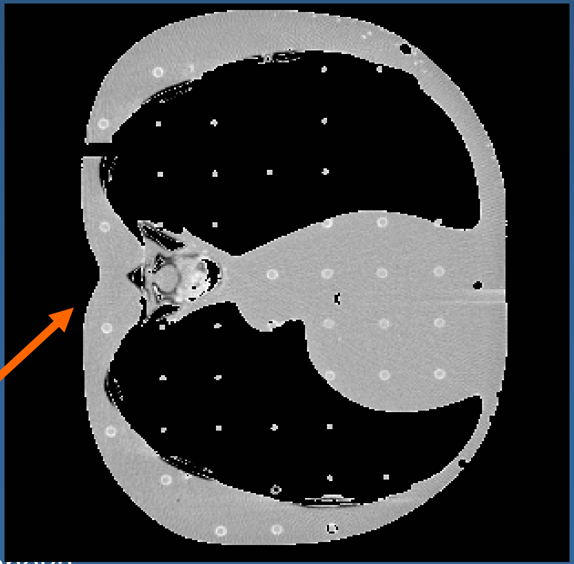
$$\chi^2/ndf \ (GEANT\ 4) = 0.52$$
$$\chi^2/ndf \ (TMS) = 0.81$$
$$\chi^2/ndf \ (PLATO) = 6.71$$

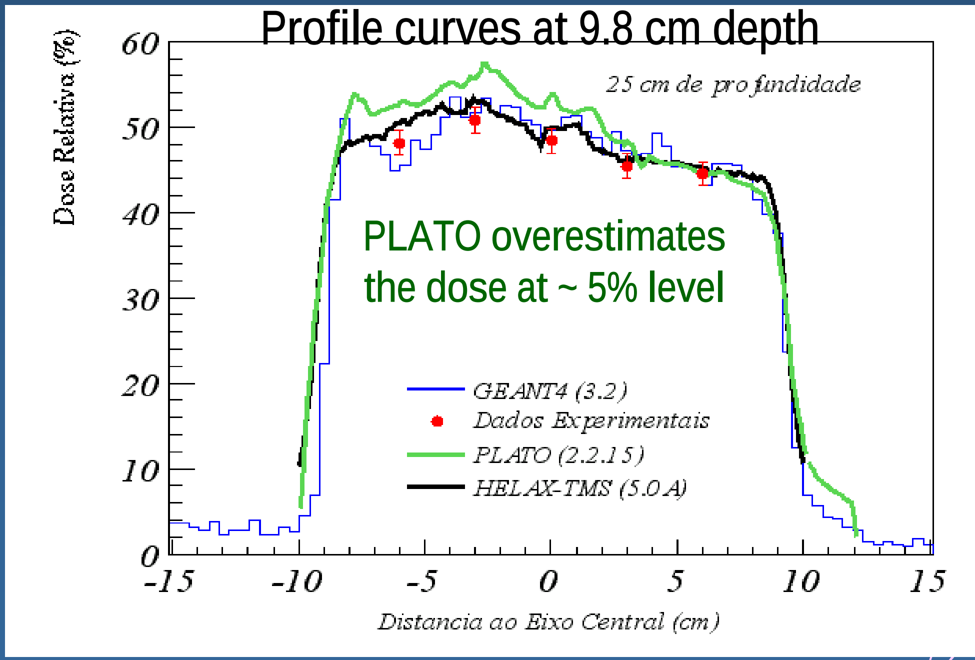


CT-simulation with a Rando phantom
Experimental data with TLD LiF dosimeter

CT images used to define the geometry:

a thorax slice from a Rando anthropomorphic phantom





Speed of Monte Carlo simulation

Speed of execution is often a concern in Monte Carlo simulation

Often a trade-off between precision of the simulation and speed of execution

Typical use cases

Semi-interactive response

- Detector design
- Optimisation
- Oncological radiotherapy

Very long execution time

- High statistics simulation
- High precision simulation

Methods for faster simulation response ⇒

Fast simulation

Variance reduction techniques (event biasing)

Inverse Monte Carlo methods

Parallelisation

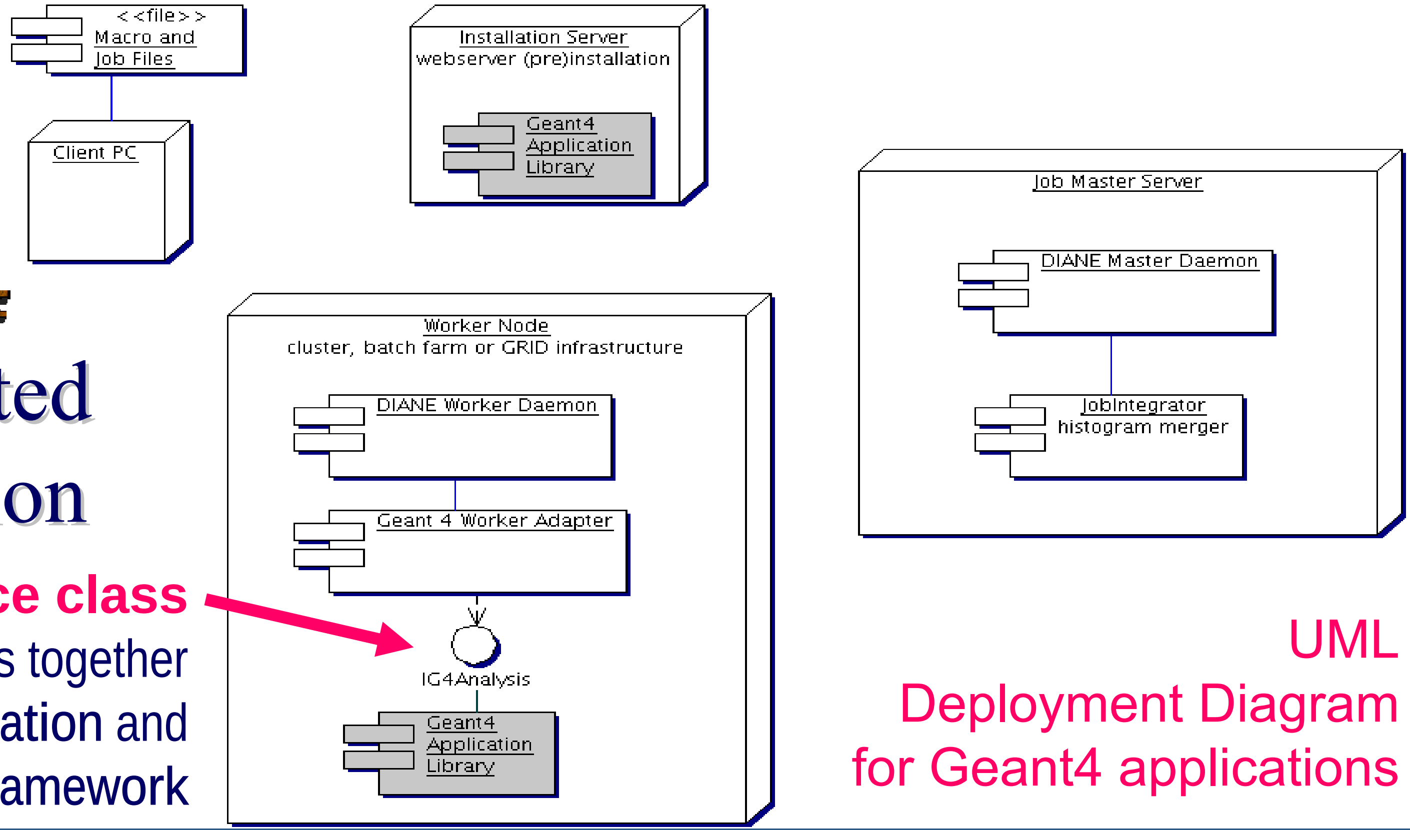
Access to distributed computing

DIANE

Transparent access
to a distributed computing environment

Parallelisation | Access to the GRID

- Required production of *Brachytherapy*: 20 M events
- 20 M events in sequential mode:16646 s (~ 4h 38’)
  on an Intel ® Pentium IV, 3.00 GHz
- The same simulation runs in 5’ in parallel on 56 CPUs
  – appropriate for clinical usage



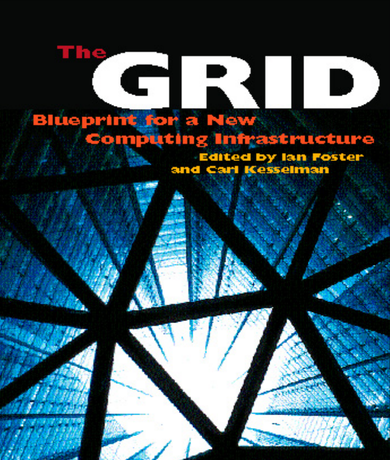
Geant 4 Distributed Simulation

Interface class which binds together Geant4 application and Master-Worker framework

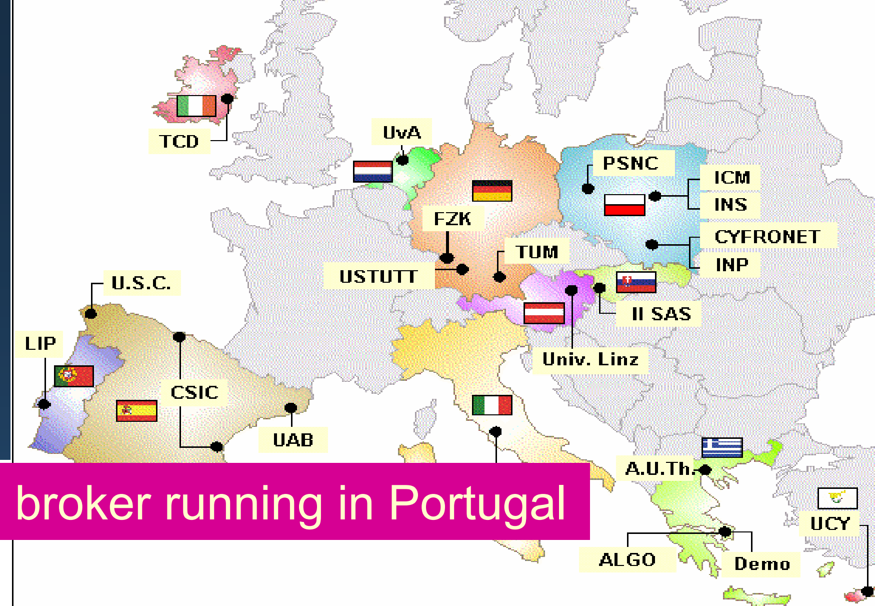
UML Deployment Diagram for Geant4 applications

Original Geant4 application source code unmodified

G4Simulation class responsible of managing the simulation
random number seeds
Geant4 initialisation
termination



Traceback from a run on CrossGrid testbed



Current #Grid setup (computing elements):

Resource broker running in Portugal

5000 events, 2 workers, 10 tasks (500 events each)

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

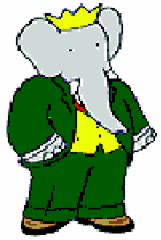
Spain

Greece

Poland

Portugal

Robustness



BaBar Simulation Production

BaBar simulation production – a millennium of work in under a year.

D. A. Smith, D. Andreotti, F. Blanc, C. Bozzi, A. Khan
for the BaBar computing group.

IEEE 2004 - Oct. 21, 2004

The Geant 4 kit

- Code
  - ~1M lines of code
  - continuously growing
  - publicly downloadable from the web
- Documentation
  - 5 manuals
  - publicly available from the web
- Examples
  - distributed with the code
  - various complete applications of (simplified) real-life experimental set-ups

- Platforms
  - Linux, SUN, Windows, (MacOS)
- Commercial software
  - None required
  - Can be interfaced
- Free software
  - CVS
  - gmake, g++
  - CLHEP
- Graphics & (G)UI
  - OpenGL, X11, OpenInventor, DAWN, VRML...
  - OPACS, GAG, MOMO...
- Persistency
  - it is possible to run in transient mode
  - in persistent mode use a HepDB interface, ODMG standard

Geant4 Collaboration

MoU based

Development, Distribution and User Support of Geant4

Major physics laboratories:

CERN, KEK, SLAC, TRIUMF

European Space Agency:

ESA

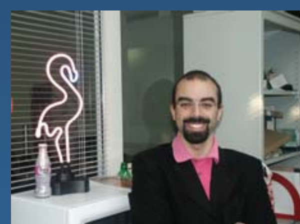
National Institutes:

INFN, IN2P3, PPARC

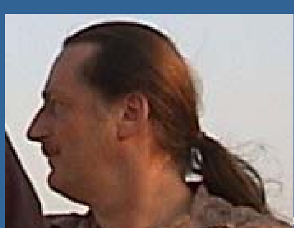
Universities:

Frankfurt Univ., Helsinki Univ., Lebedev Inst., LIP, *etc.*

21-121 members in the RD44 phase, ~ 60 currently




COMUNITA'



The next frontier

The power of abstract interfaces

Geant4-DNA - Microsoft Internet Explorer

File Edit View Favorites Tools Help

Back Search Favorites Media

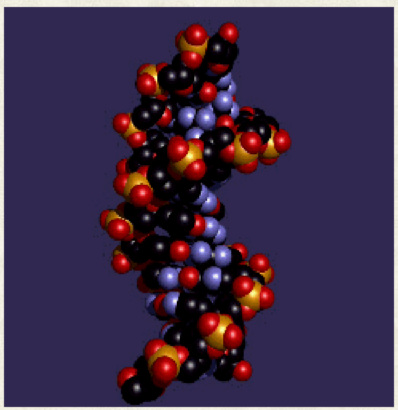
Address D:\Users\pia\wwwG4infn\dna\index.html Go Links

Geant 4 DNA

INFN Istituto Nazionale di Fisica Nucleare

- Home
- Requirements
- 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

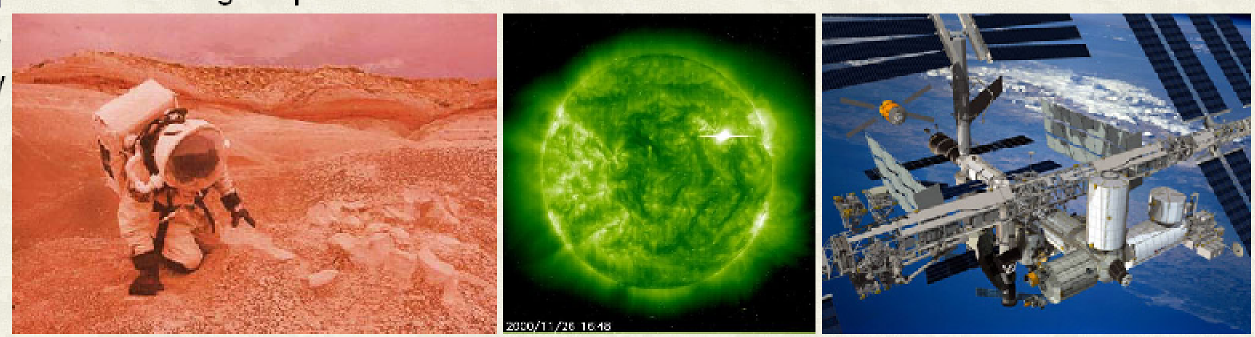


Estimating **cancer risk for human exposures to space radiation** is a challenge which involves a wide range of knowledge in physics, chemistry, biology and medicine.

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.

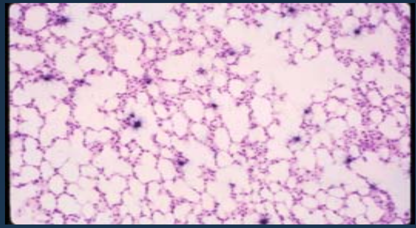
A novel approach, based on the new-generation object-oriented Geant4 Monte Carlo Toolkit, proceeds in a reverse order, from bottom to top, by analysing the nano-scale effects of energetic particles at the cellular and DNA molecule level.

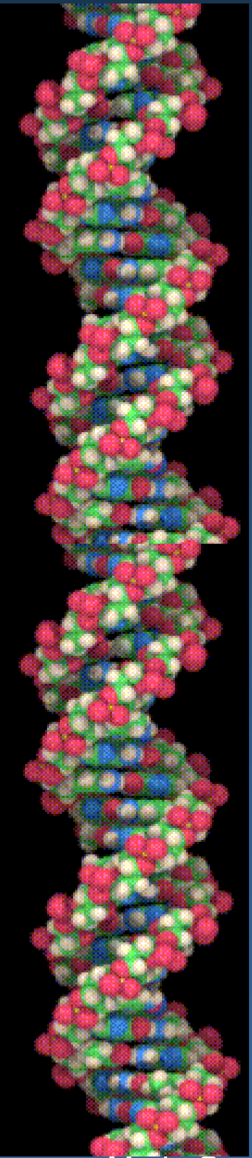
This project is sponsored by the European Space Agency (ESA) and is pursued by a multidisciplinary European team of biologists, physicians, physicists, space scientists and software engineers.



Pictures courtesy of ESA

Geant 4 for radiation biology





- Several specialized Monte Carlo codes have been developed for radiobiology/microdosimetry
  - Typically each one implementing models developed by its authors
  - Limited application scope
  - Not publicly distributed
  - Legacy software technology (FORTRAN, procedural programming)
- Geant4-DNA
  - Full power of a general-purpose Monte Carlo system
  - Toolkit: multiple modeling options, no overhead *(use what you need)*
  - Versatility: from controlled radiobiology setup to real-life ones
  - Open source, publicly released
  - Modern software technology
  - Rigorous software process

Low Energy Physics extensions

DNA level

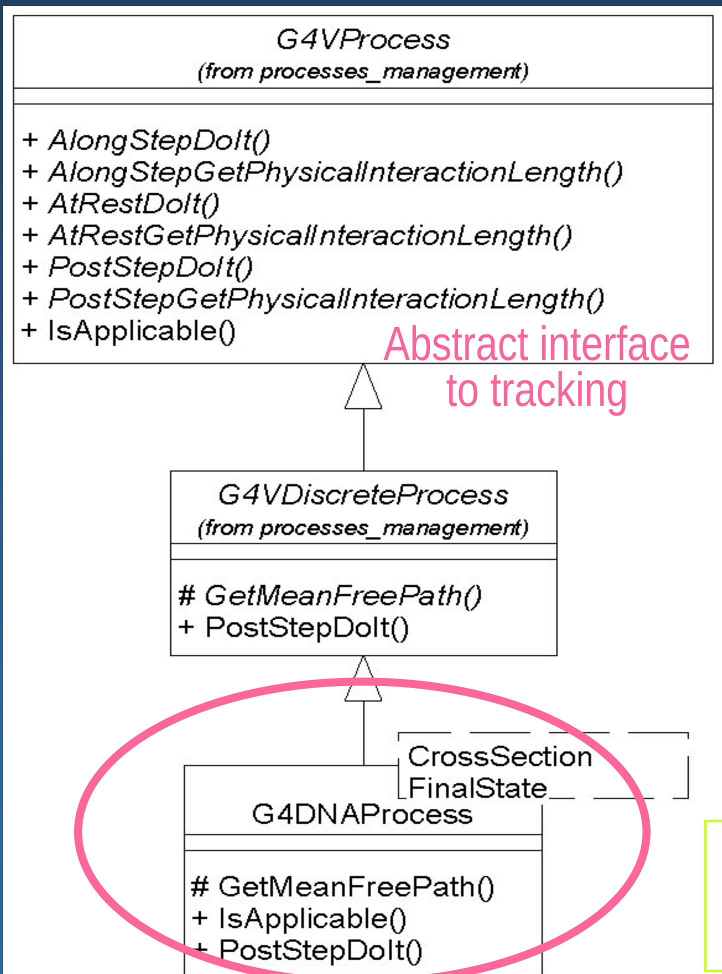
- Specialised processes down to the eV scale
  - at this scale physics processes depend on the detailed atomic/molecular structure of the medium
  - 1st cycle: processes in water
- Releases
  - β-version in Geant4 8.1 (June 2006)
  - Refined version in progress
  - Further extensions to follow
- Processes for other materials to follow
  - interest for radiation effects on components

Particle	Processes
e	Elastic scattering Excitation Ionisation
p	Excitation Charge decrease Ionisation
H	Charge increase Ionisation
He++	Excitation Charge decrease Ionisation
He+	Excitation Charge decrease Charge increase Ionisation
He	Excitation Charge increase Ionisation

Software design

Innovative design introduced in Geant4: **policy-based class design**

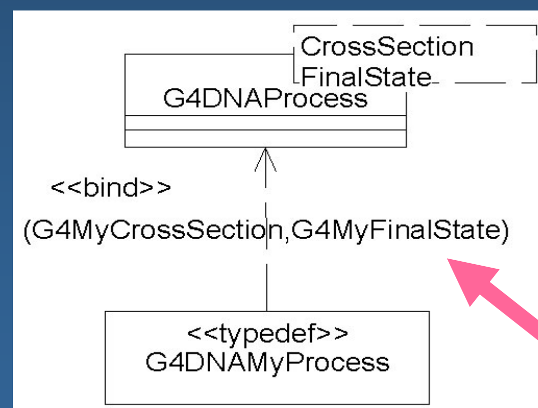
Flexibility of modeling + performance optimisation

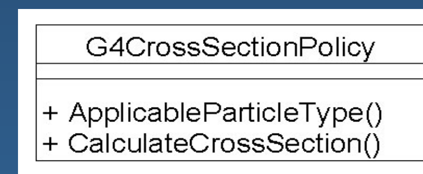


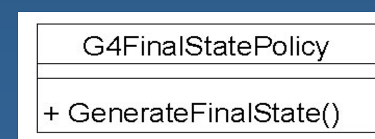
Parameterised class

Policies

- cross section calculation
- final state generation







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

Policy based design

- Policy based classes are parameterised classes
  - classes that use other classes as a parameter
- Specialization of processes through template instantiation
  - The code is bound at compile time
- Advantages
  - Policies are not required to inherit from a base class
  - 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
  - No need of virtual methods, resulting in faster execution
- Clean, maintainable design of a complex domain
  - Policies are orthogonal
- Open system
  - Proliferation of models in the same environment

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 testing in parallel with implementation

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.

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.

B. Grosswendt and E. Waibel, "Transport of low energy electrons in nitrogen and air", Nucl. *Instrum. Meth.*, vol. 155, pp. 145-156, 1978.

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.

D. Emfietzoglou, and M. Moscovitch, "Inelastic collision characteristics of electrons in liquid water", *Nucl. Instrum. Meth. B,* vol. 193, pp. 71-78, 2002.

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.

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.

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.

J. H. Miller and A. E. S. Green, "Proton Energy Degradation in Water Vapor", *Rad. Res.*, vol. 54, pp. 343-363, 1973.

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.

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 H2O: absolute differential and integral cross sections", *Phys. Rev. A,* vol. 55, no. 5, pp. 3945-3946, 1997.

K. H. Berkner, R. V. Pyle, and J. W. Stearns, "Cross sections for electron capture by 0.3 to 70 keV deuterons in H2, H2O, CO, CH4, and C8F16 gases" , *Nucl. Fus.*, vol. 10, pp. 145-149, 1970.

R. Dagnac, D. Blanc, and D. Molina, "A study on the collision of hydrogen ions H1+, H2+ and H3+ with a water-vapour target", *J. Phys. B: Atom. Molec. Phys.*, vol. 3, pp.1239-1251, 1970.

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.

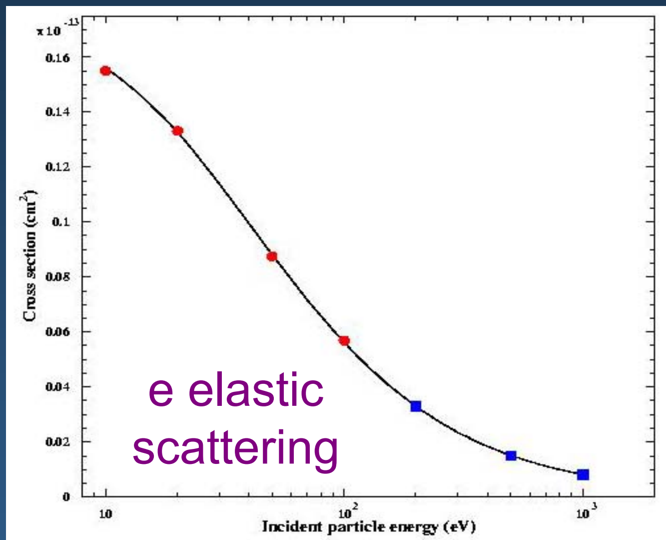
P. G. Cable, Ph. D. thesis, University of Maryland, 1967.

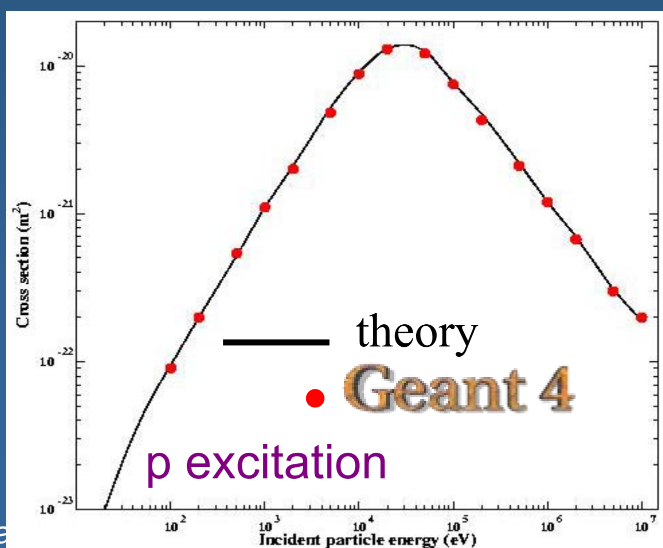
M. E. Rudd, T. V. Goffe, R. D. DuBois, L. H. Toburen, "Cross sections for ionisation of water vapor by 7-4000 keV protons", *Phys. Rev. A*, vol. 31, pp. 492-494, 1985.

Test

Verification

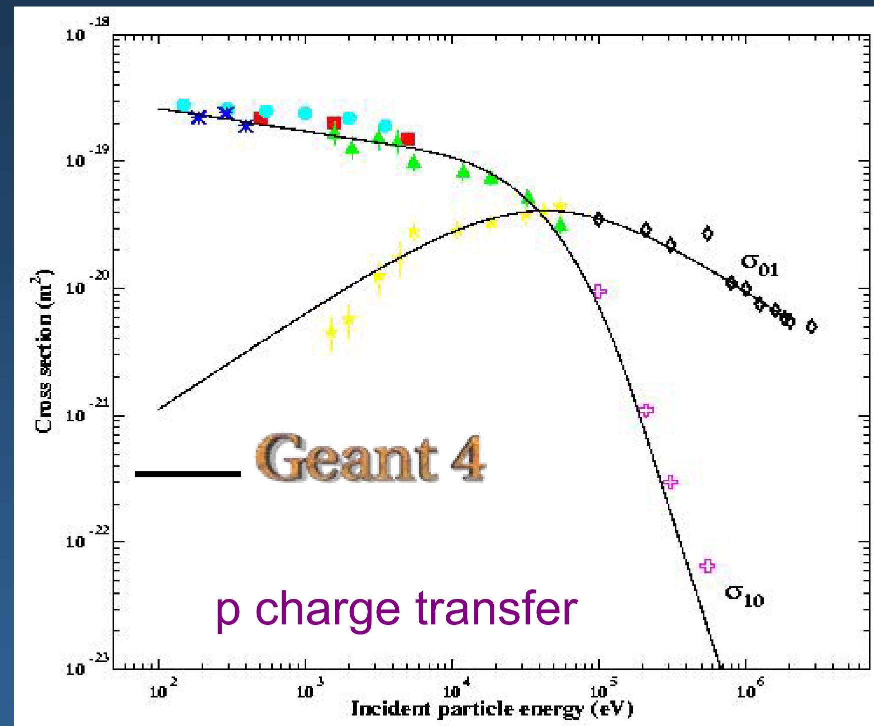
against theoretical models





Comparison

against experimental data



Scarce experimental data

Large scale validation project planned

TARGET THEORY	SINGLE-HIT	$S = e^{-D / D_0}$
TARGET THEORY	MULTI-TARGET SINGLE-HIT	$S = 1 - (1 - e^{-qD})^n$ REVISED MODEL: $S = e^{-q_1 D} \, [\, 1 - (1 - e^{-q_n D})^n \,]$
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	$S = e^{-\alpha D}[1 + (\alpha D T / \varepsilon)]^{\varepsilon}$
MOLECULAR THEORY	REPAIR-MISREPAIR LIN REP / MIS	$S = e^{-\alpha D}[1 + (\alpha D / \varepsilon)]^{\varepsilon \Phi}$
MOLECULAR THEORY	LETHAL-POTENTIALLY LETHAL	$S = \exp\left[- N_{TOT}\left[1 + \frac{N_{PL}}{\varepsilon\,(1 - e^{-\varepsilon B A t r})}\right]^{\varepsilon} \right]$
MOLECULAR THEORY	LETHAL-POTENTIALLY LETHAL – LOW DOSE	$S = e^{-\eta_{AC} D}$
MOLECULAR THEORY	LETHAL-POTENTIALLY LETHAL – HIGH DOSE	$-\ln[S(t)] = (\eta_{AC} + \eta_{AB})\, D - \varepsilon \ln[1 + (\eta_{AB} D/\varepsilon)(1 - e^{-\varepsilon B A\, tr})]$
MOLECULAR THEORY	LETHAL-POTENTIALLY LETHAL – LQ APPROX	$-\ln[S(t)] = (\eta_{AC} + \eta_{AB}\, e^{-\varepsilon B A tr})\, D + (\eta^2_{AB}/2\varepsilon)(1 - e^{-\varepsilon B A\, tr})^2 D^2]$

In progress

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

Geant4 approach:
variety of models all handled
through the same abstract
interface

in progress

Geant 4

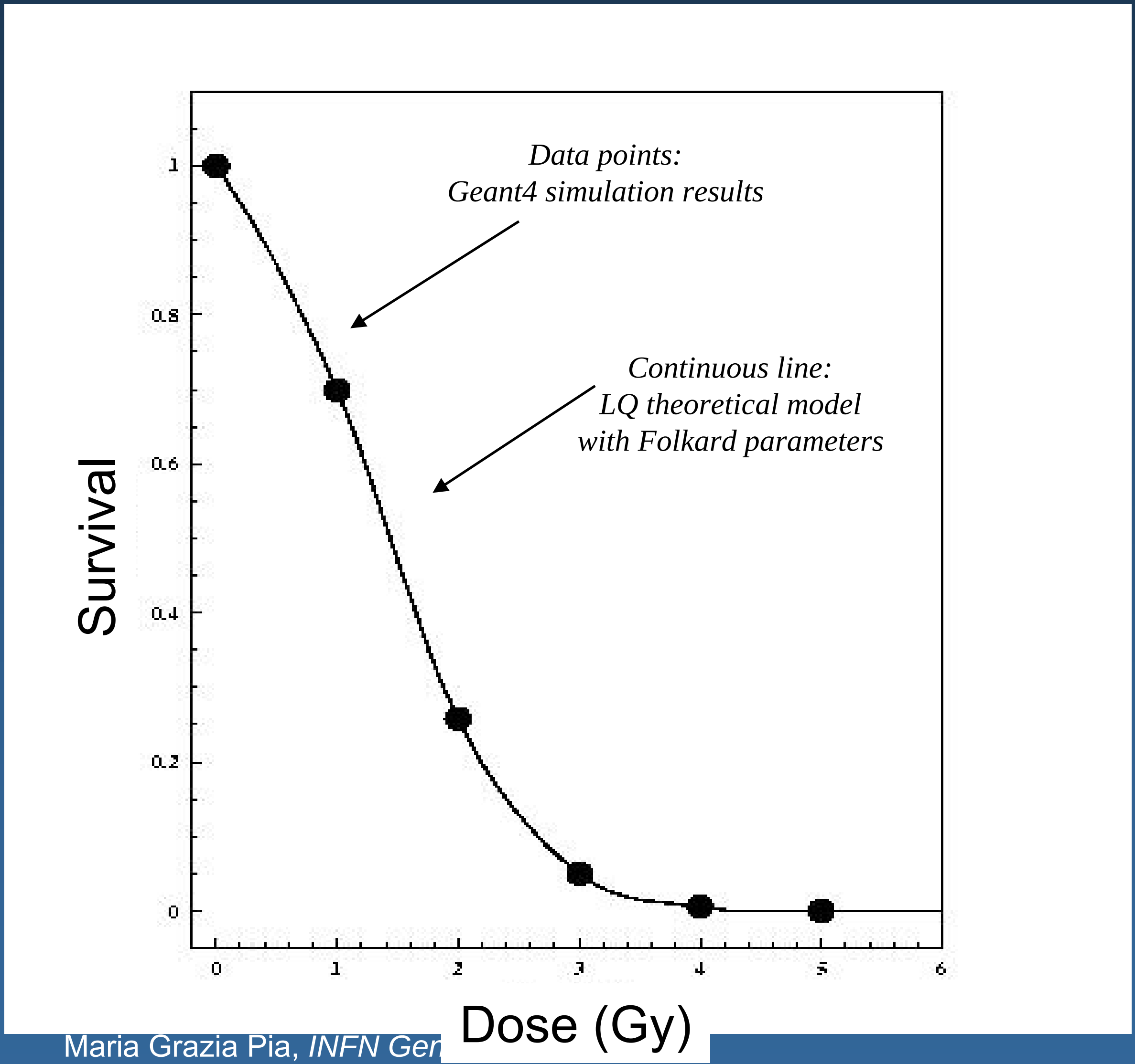
Analysis & Design
Implementation
Test

Requirements
Problem domain analysis

Incremental-iterative
software process

Experimental validation of
Geant4 simulation models

Cell survival models verification



Monolayer

V79-379A cells

Proton beam
E= 3.66 MeV/n

LQ model

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

$\alpha = 0.32$
$\beta = -0.039$

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

Geant 4 for medicine

- Macroscopic
  - calculation of dose
  - medical imaging
  - 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
  - processes for DNA strand breaking, repair etc.

Complexity of

software, physics and biology

addressed with an iterative and incremental software process

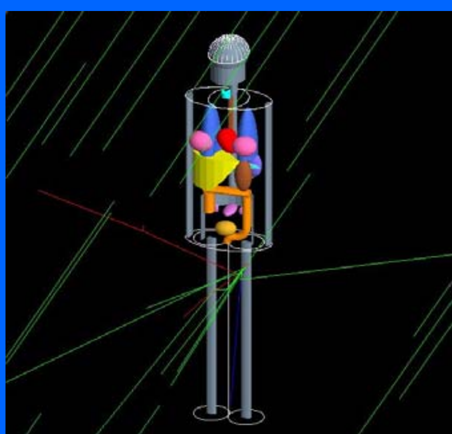
↓

Parallel development at all the three levels

(domain decomposition)

Scenario for Mars and hospitals

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



Dose in organs at risk

Phase space input to nano-simulation

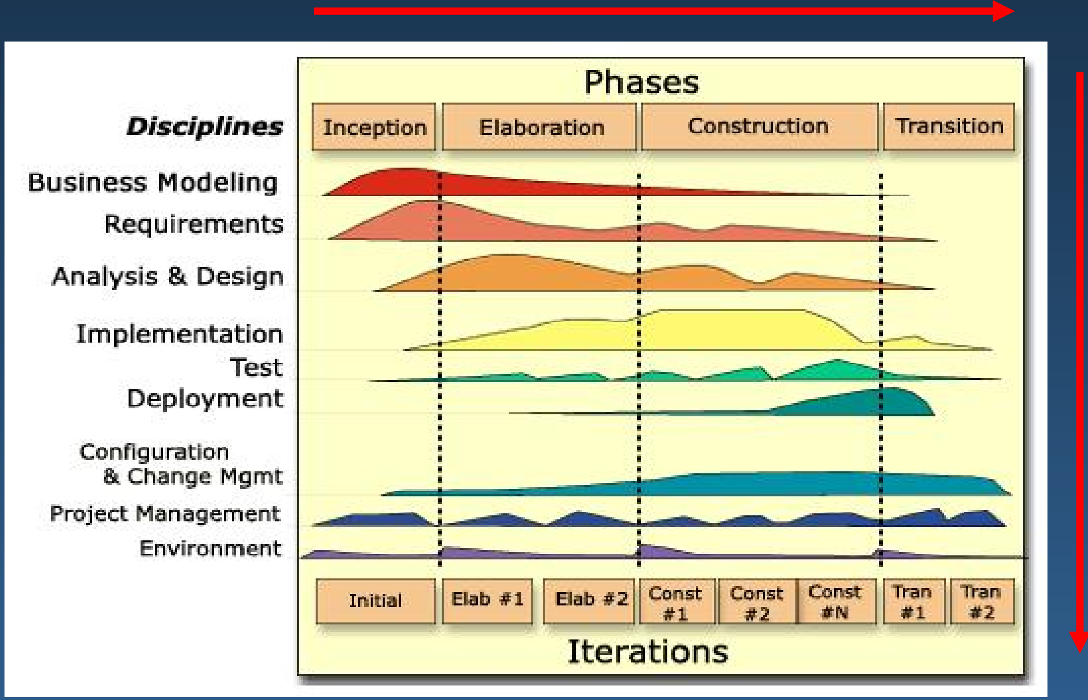
Geant4 simulation with biological processes at cellular level (cell survival, cell damage…)

Oncological risk to astronauts/patients

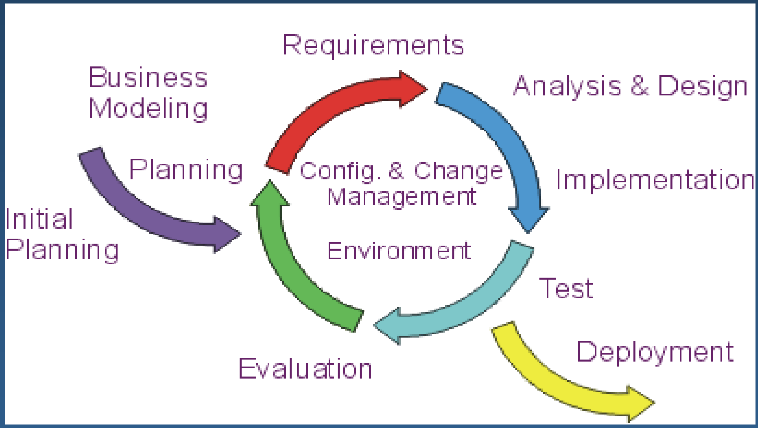
Risk of nervous system damage

Geant4 simulation with physics at eV scale
+
DNA processes

…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

Conclusions

Complexity of physics, detectors, environments

A rapidly changing computing environment

Similar requirements across diverse fields (HEP, astrophysics, medicine…)

The response:

- rigorous approach to software engineering
- OO technology
- powerful functionality, rich physics

Achieve:

- openness to extension and evolution
- maintainability over an extended time scale
- transparency of physics

Results:

- HEP, space science, medical physics…
- science + technology transfer