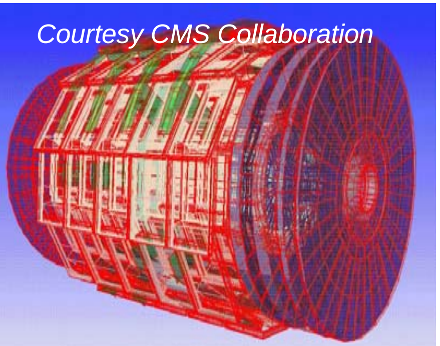
Geant 4

for microdosimetry

Radiobiology, nanotechnology, radiation effects on components

S. Chauvie *(Cuneo Hospital and INFN Genova)*
Maria Grazia Pia (INFN Genova)

Workshop: La radiobiologia dell'INFN
Trieste, 7 February 2008



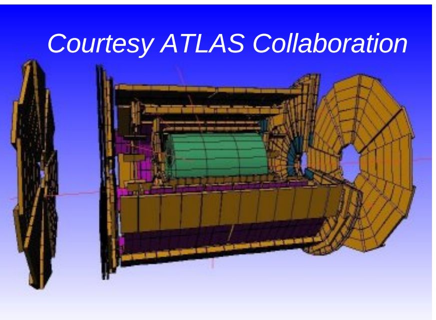
Geant 4

S. Agostinelli et al.
GEANT4 - a simulation toolkit
NIM A 506 (2003) 250-303

Most cited (>132000 papers)
"Nuclear Science and Technology" publication!

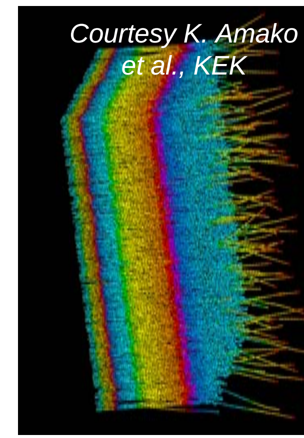
3rd most cited INFN paper

Born from the requirements of large scale HEP experiments

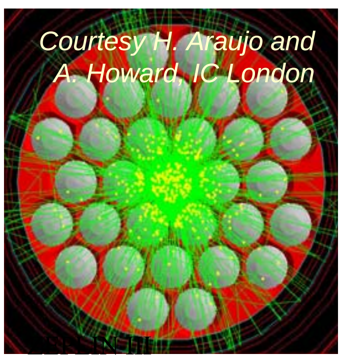


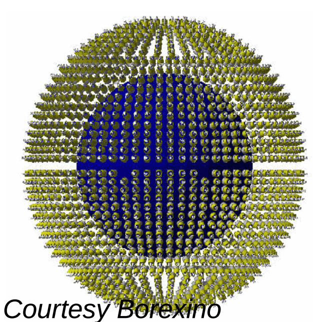
Widely used also in

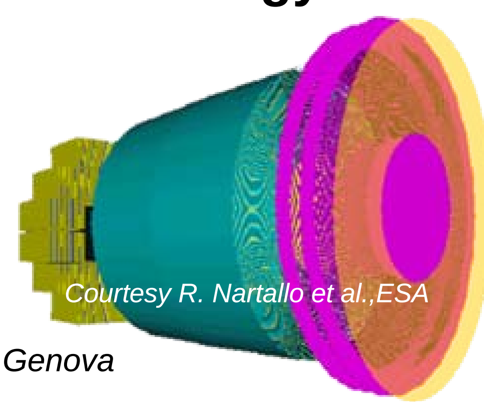
- Space science and astrophysics
- Medical physics, nuclear medicine
- Radiation protection
- Accelerator physics
- Humanitarian projects, security
- etc.

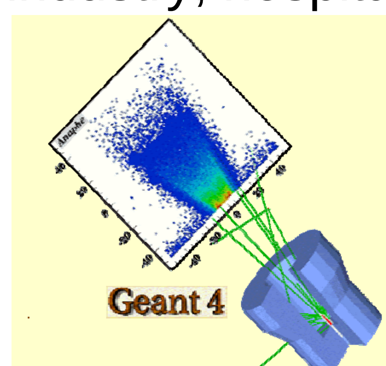


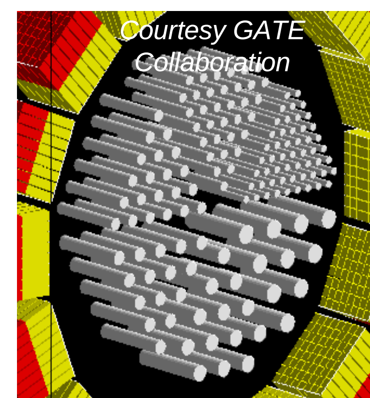
Technology transfer to industry, hospitals…











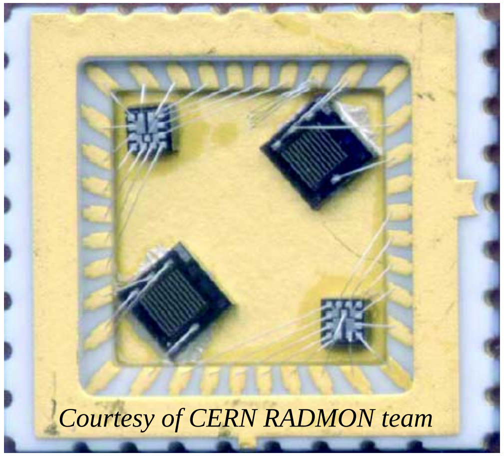
INFN Genova

Multi-disciplinary application environment

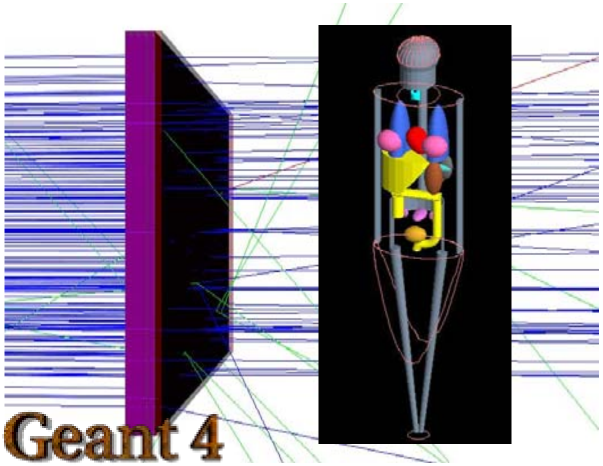
Dosimetry

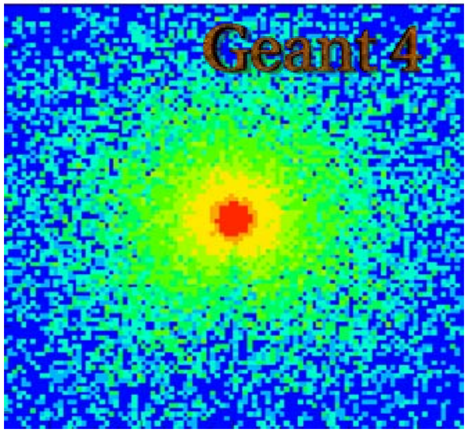
Space science

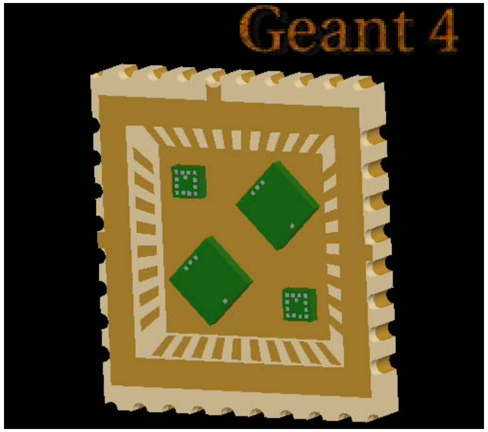
Radiotherapy



Effects on components







Wide spectrum of physics coverage, variety of physics models

Precise, quantitatively validated physics

Accurate description of geometry and materials

Geant 4 — **Multiple** domains in the **same** software environment

- **Macroscopic level**
  - calculation of dose
  - already feasible with Geant4
  - develop useful associated tools
- **Intermediate level**
  - statistical models
  - processes for cell survival, damage etc.
- **Microscopic level**
  - physics processes at the eV scale
  - bio-chemical processes etc.

Complexity of

software, physics and biology

addressed with an iterative and incremental software process

↓

Parallel development at all the three levels

(domain decomposition)

Orticultura

What's new in Geant4?

- **Many "track structure" Monte Carlo codes previously developed**
  – A lot of modelling expertise embedded in these codes
  – Each code implements one modelling approach (developed by its authors)
  – "Stand-alone" codes, with limited application scope
  – Legacy software technology (FORTRAN, procedural programming)
  – Not publicly distributed

- **Geant4**
  – "Track structure" simulation in a **general-purpose** Monte Carlo system
  – **Toolkit** approach: many interchangeable models *(no emotional attachment to any)*
  – Advanced **software technology**
  – Rigorous **software process**
  – **Open source**, freely available, supported by an international organization
  – Foster a **collaborative** spirit in the scientific community
  – Benefit of the **feedback** of a wider user community

Geant 4 DNA

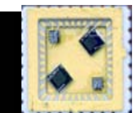
INFN *Genova – Partly sponsored by ESA*

Sub-domain of
Geant4 Low-Energy Electromagnetic Physics
Follows the same rigorous software standards

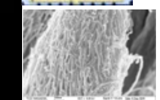
Not only…

rather…

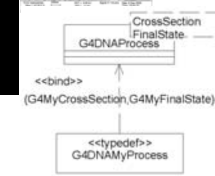
Dosimetry
Nanotechnology
Architecture



Courtesy of RADMON, CERN



Courtesy of A. Montanari, INFN BO



Radiobiology
Radiation effects on components
Nanotechnology-based detectors

Commonality
across experimental domains

Physics issues
Models depend on the detailed dielectric structure of the interacting material

Computational stress
CPU-intensive simulation for tracks at the nm scale

Solution
Commonality-differentiation

Technology
New software design technique first introduced in Monte Carlo

Modelling
Multiple implementations
No "one size fits all" in this domain

1st development cycle: Geant4 physics extensions

Physics of interactions in water down to the eV scale

- **Complex domain**
  - **Physics**: collaboration with theorists
  - **Technology**: innovative design technique introduced in Geant4 (1st time in Monte Carlo)
- **Experimental complexity** as well
  - Scarce experimental data
  - Collaboration with experimentalists for model validation
  - Geant4 physics validation at low energies is difficult!

S. Chauvie et al., Geant4 physics processes for microdosimetry simulation: design foundation and implementation of the first set of models, IEEE Trans. Nucl. Sci., Vol. 54, no. 6, pp. 2619-2628, Dec. 2007

Geant4-DNA physics processes

Specialised processes for low energy interactions with water

- **Models in liquid water**
  - More realistic than water vapour
  - Theoretically more challenging
  - Hardly any experimental data
  - New measurements needed
- **Status**
  - 1st β-release Geant4 8.1 2006
  - Full release December 2007
  - Further extensions in progress
- **Current focus**
  - Experimental comparisons

Toolkit: *offer a wide choice among available alternative models for each process*

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

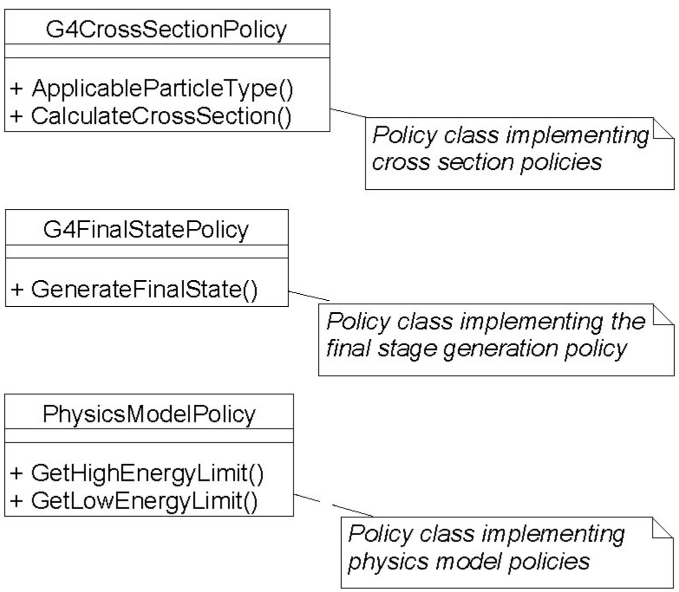
What is behind… **Policy-based class design**

- A policy defines a class or class template interface
- Policy host 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
  - The code is bound at compilation time
    - No need of virtual methods, resulting in faster execution

New technology

1st time introduced in Monte Carlo

Technology motivated by scientific requirements!



Weak dependency of the policy and the policy based class on the policy interface

Syntax-oriented rather than signature-oriented

Highly **customizable** design

Open to extension

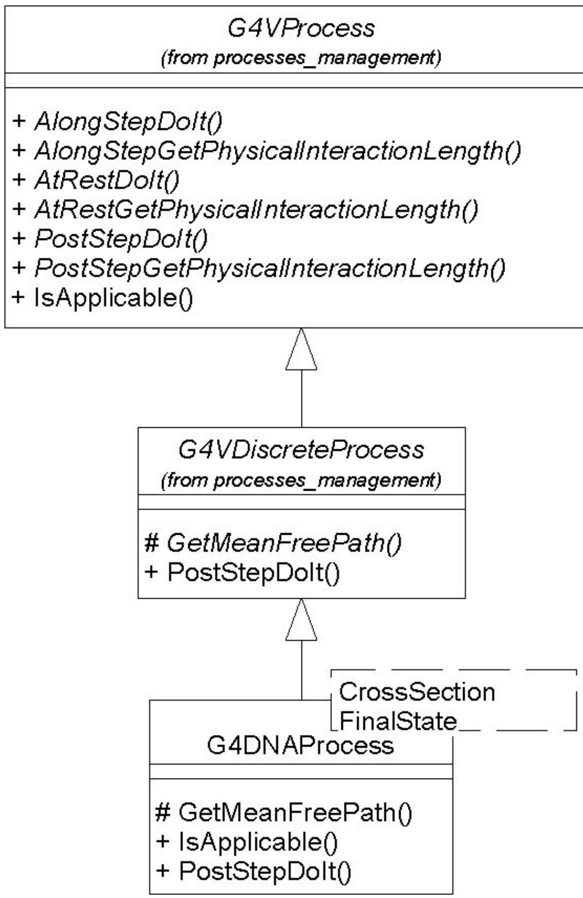
Policies can proliferate w/o any limitation

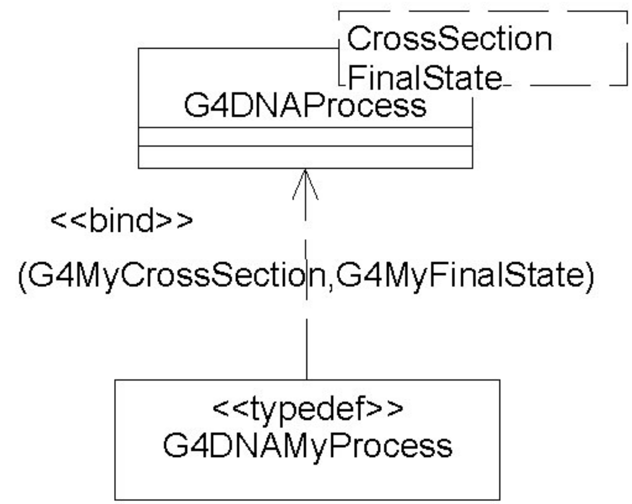
Geant4-DNA physics process

Handled transparently by Geant4 kernel

Deprived of any intrinsic physics functionality

Configured by **template specialization** to acquire physics properties





Development metrics

- Open to extension: what does it mean in practice?
- Implementation + unit test of a new physics model
  - ~ 5 to 7 hours* (low level C++ programming experience)
  - **No integration effort at all**

Investment in
software technology!

**...provided theorists have previously done their job by doing the theoretical calculation!*

How **accurate** are Geant4-DNA physics models ?

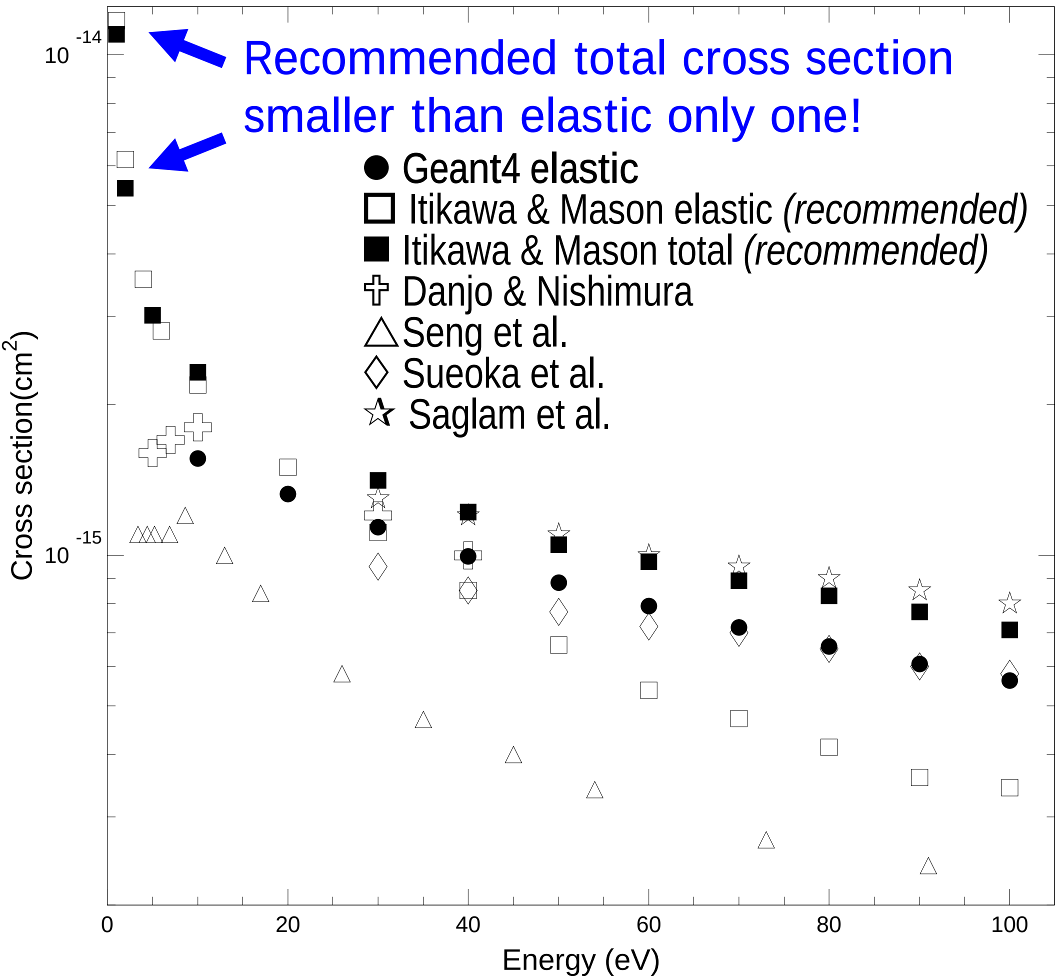
- Both theoretical and experimental complexity in the very low energy régime

- Theoretical calculations must take into account the detailed dielectric structure of the interacting material
  - Approximations, assumptions, semi-empirical models

- Experimental measurements are difficult
  - Hardly any experimental data in liquid water
  - Control of systematics, experimental constraints depending on the phase
- Evaluation of **plausibility**
  - Only practical option at the present stage
  - Comparison against experimental data in water vapour/ice
  - Interesting also to study phase-related effects

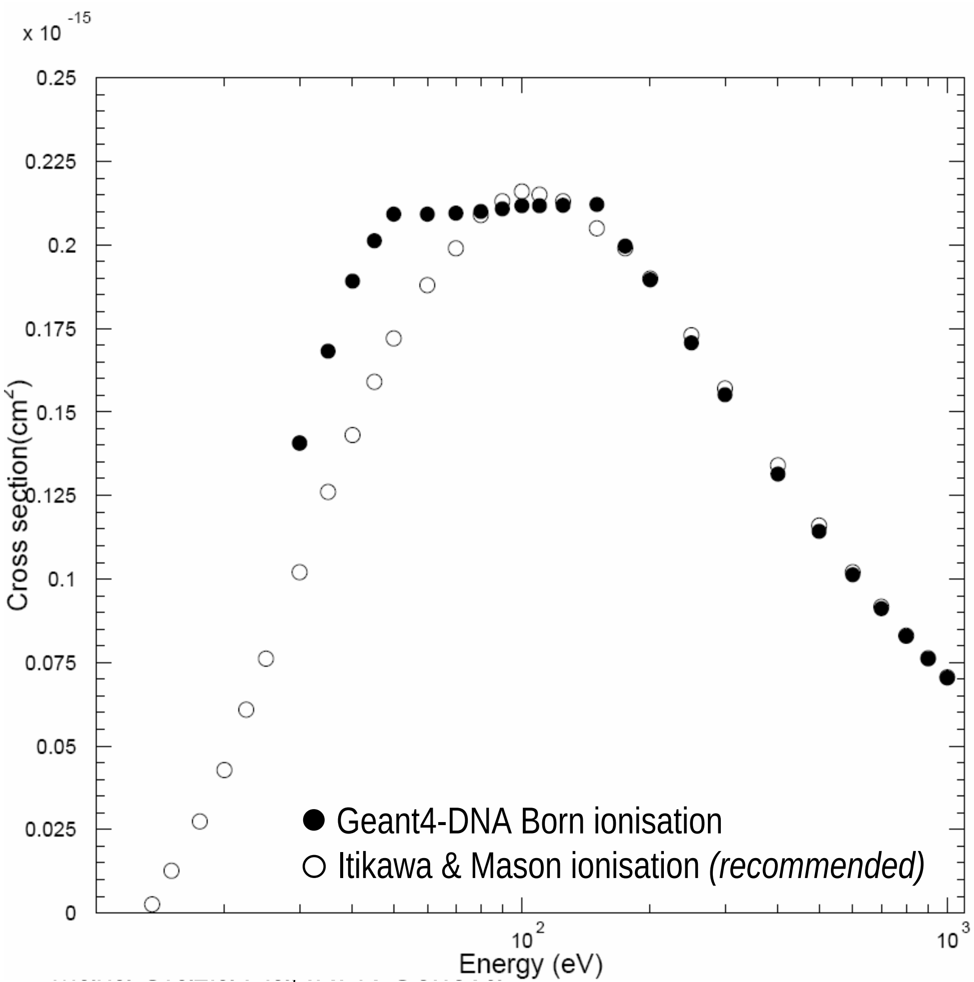
Electron elastic scattering: total cross section

Not all available experimental data reported…
the picture would be too crowded!



- **Evident discrepancy of the experimental data**
- **Puzzle:** inconsistency in recommended evaluated data from *Itikawa & Mason, J. Phys. Chem. Ref. Data, 34-1, pp. 1-22, 2005.*
- Geant4
  - Better agreement with some of the data sets
  - Hardly conclusive comparison, given the experimental status…

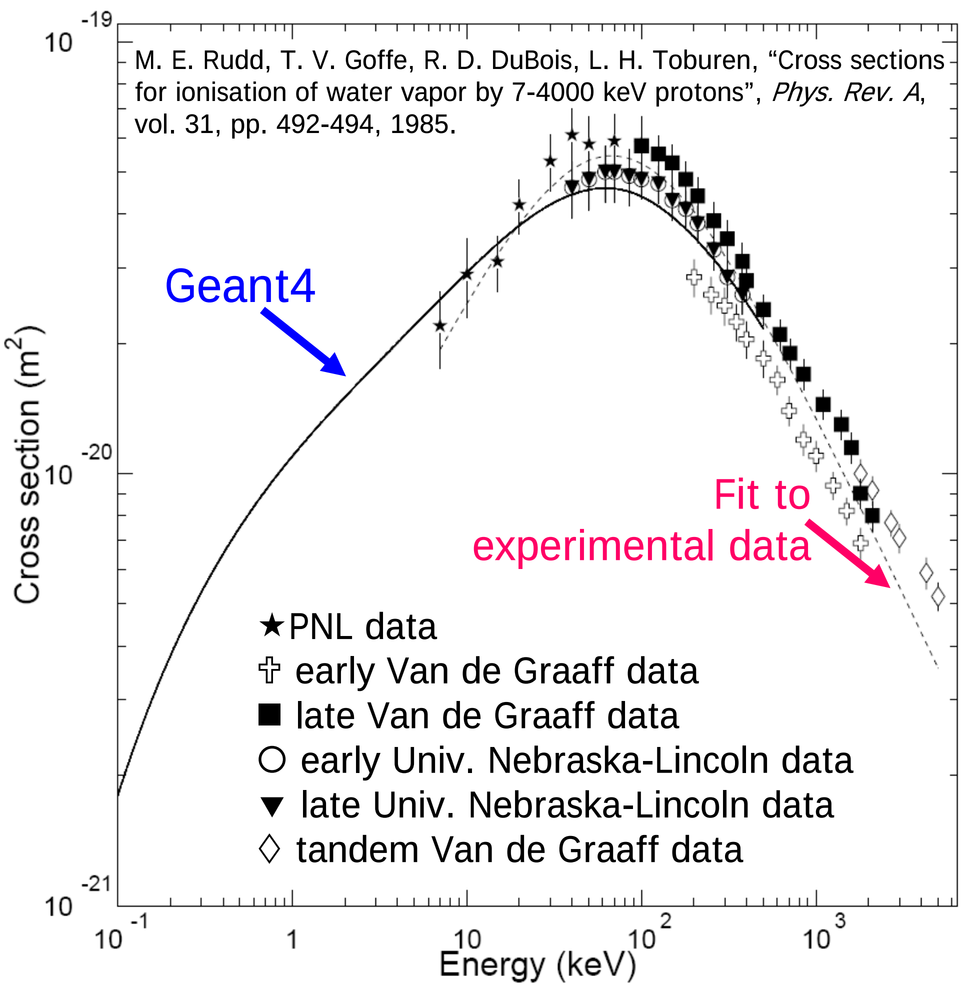
Electron ionisation: total cross section



- Different phases
  - Geant4-DNA model: liquid water
  - Experimental data: vapour
- **Plausible** behaviour of Geant4 implementation
- Phase differences appear more significant **at lower energies**

Proton ionisation: total cross section

Different phases
Geant4 model: liquid water
Experimental data: vapour

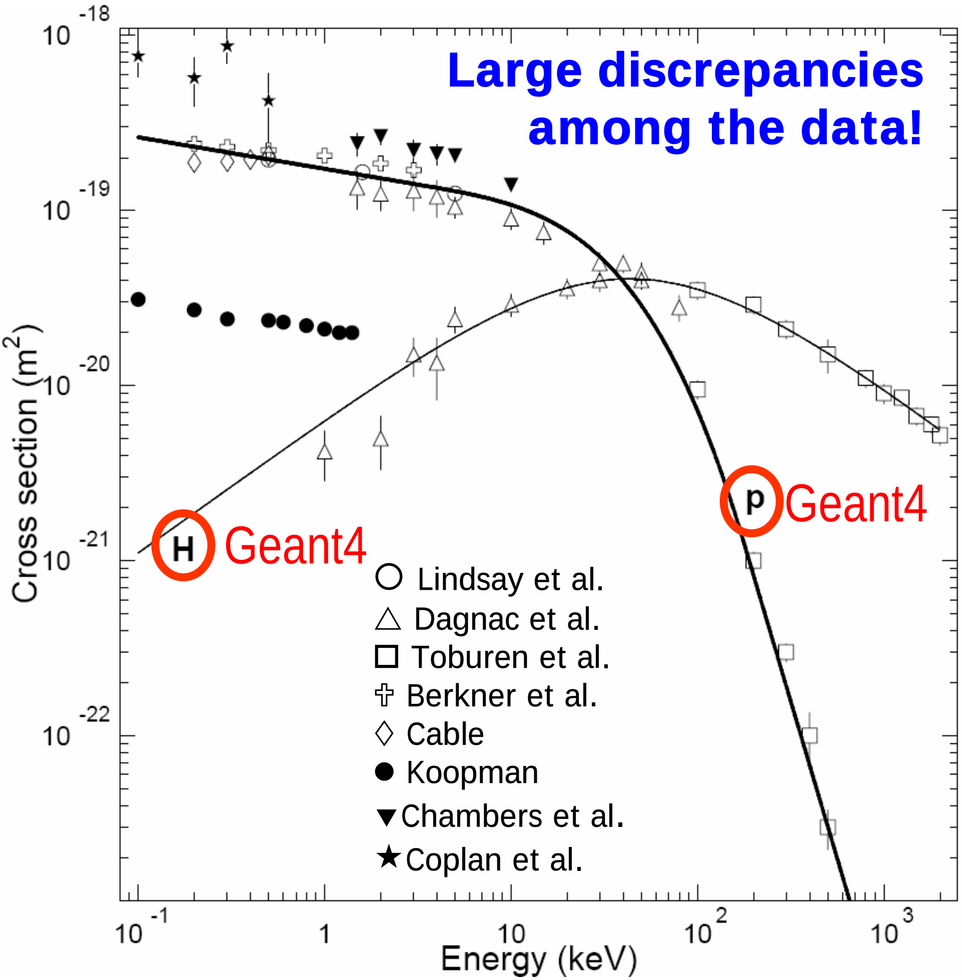


- All measurements performed by the same team
  - at different accelerators and time
- Even data taken by the same group exhibit inconsistencies !
  - systematic is difficult to control in delicate experimental conditions
- Geant4 models look **plausible**
- Hard to discuss **phase effects** in these experimental conditions!
- **Goodness-of-fit test**
  - Geant4 model incompatible with experimental data (*p-value* < 0.001)
  - Compatibility w.r.t. data fit?

    Cramer-von Mises test: *p-value* $= 0.1$

    Anderson-Darling test: *p-value* < 0.001

Charge change cross section: proton and hydrogen



- Different phases
  - Geant4 model: liquid
  - Experimental data: vapour
- Goodness-of-fit test
  - Geant4 model
  - experimental data *(white symbols only)*
    - Anderson-Darling test
    - Cramer-von Mises test
    - Kolmogorov-Smirnov test
    - Kuiper test
    - Watson test
  - p-value > 0.1 from all tests

... but some data were used to optimise the semi-empirical model!

Conclusion from comparisons

- Geant4-DNA models (liquid) look **plausible** when compared to available experimental data (vapour)

- **More experimental data are needed**
  - In **liquid water** for simulation model validation
  - In **vapour** and **ice** to study the importance of phase effects in modelling particle interactions with the medium
  - With good **control of systematic** and **reproducibility** of experimental conditions!

- Hard to draw firm conclusions about phase effects
  - Available experimental data exhibit significant discrepancies in many cases
  - Some of these data have been already used to constrain or optimize semi-empirical models

Exploiting the toolkit

For the first time
a **general-purpose Monte Carlo** system
is equipped with functionality specific
to the simulation of
biological effects of radiation

Geant4-DNA
physics processes

+

Geant 4

Kernel

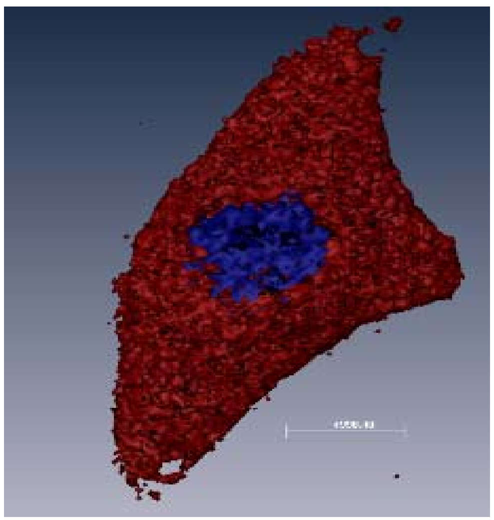
User Interface

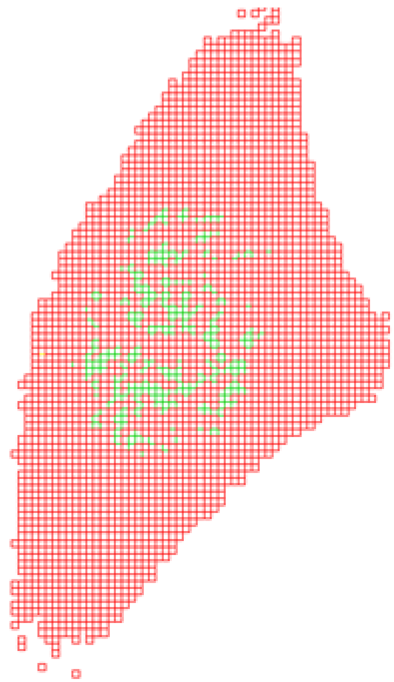
Geometry

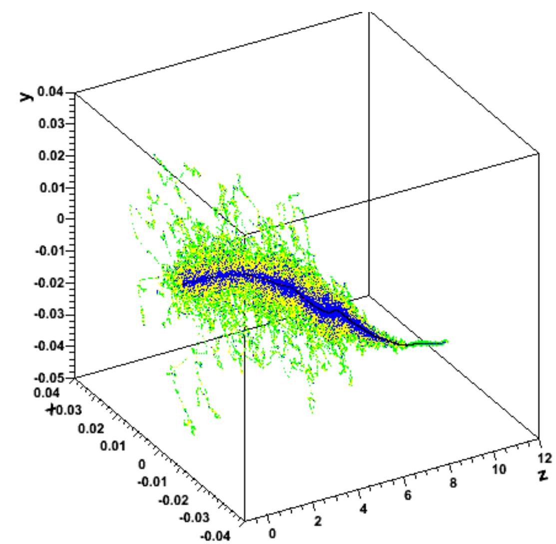
Visualisation

User application

Microdosimetry with Geant4
in high resolution cellular phantoms at CENBG



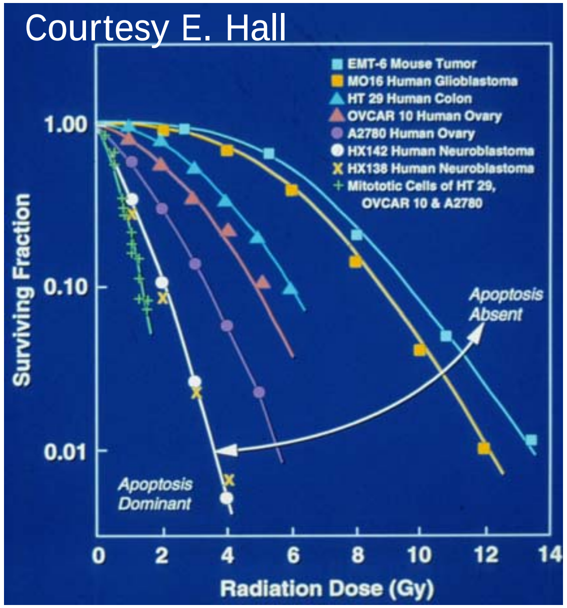




freely usable INFN original ideas,
technology and software developments
in an open-source software environment

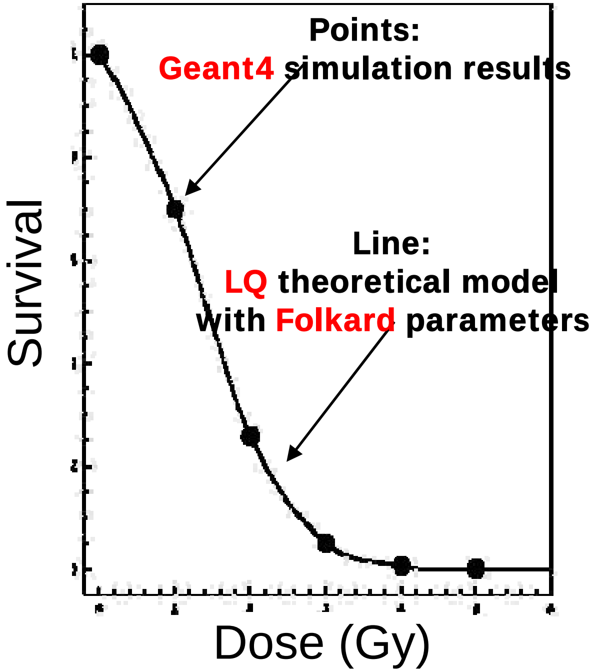
Changing scale

- Parallel approach: **macroscopic** modelling in Geant4
  - Concept of **dose** in a **cell population**
  - **Statistical** evaluation of radiation effects from **empirical data**
  - In the same simulation environment ⇒ **toolkit**



Human cell lines irradiated with X-rays

Example: modelling **cell survival fraction** in a population of irradiated cells



For discussion…

- Geant4 proposes a paradigm shift
  - Open source, freely available software
  - Microdosimetry functionality in a general-purpose Monte Carlo code
  - Availability of multiple models in the same environment
  - Equal importance to **functionality** and **software technology**
  - Foster collaboration within the scientific community
    - Theoretical modelling, experimental measurements, software technology
  - Promote feedback from users of the software
- Same environment for different research areas:
  - Radiobiology
  - Detector R&D, nanotechnology
  - Radiation effects on components, electronics
- Comments and suggestions are welcome...

Acknowledgment

- Thanks to
  - M. Dingfelder and D. Emfietzoglou for theoretical support
  - W. Friedland and H. Paretzke for fruitful discussions and suggestions
  - G. Cosmo and I. McLaren for support in the Geant4 system testing process
  - K. Amako for support in releasing the Geant4-DNA code documentation
  - Z. W. Bell (ORNL) for constructive advice
  - CERN Library for providing many reference papers