Geant4 for Microdosimetry

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on behalf of the Geant4-DNA Team
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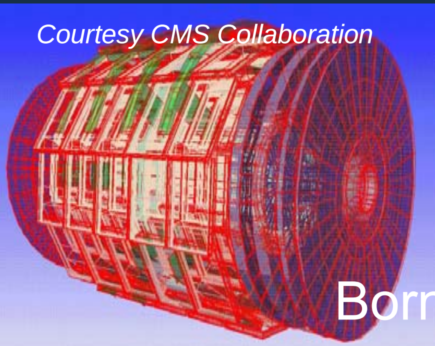
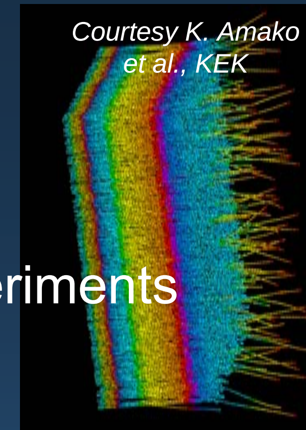
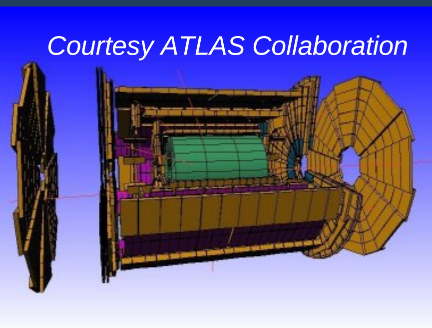
MCNEG Workshop
NPL, 28-29 March 2006

Geant 4


Courtesy CMS Collaboration

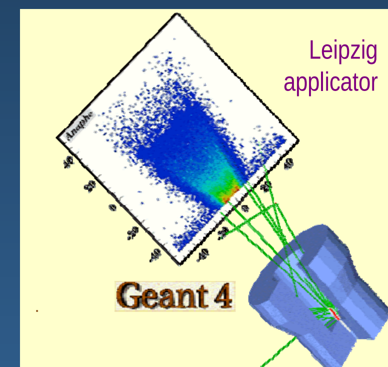

Courtesy K. Amako et al., KEK

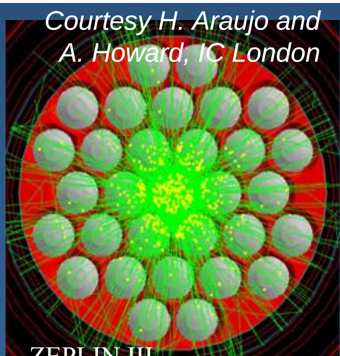
Born from the requirements of large scale HEP experiments


Courtesy ATLAS Collaboration

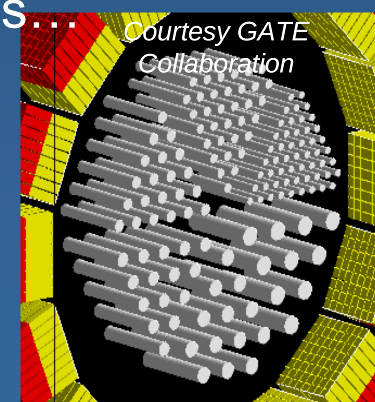
Widely used also in

- 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…



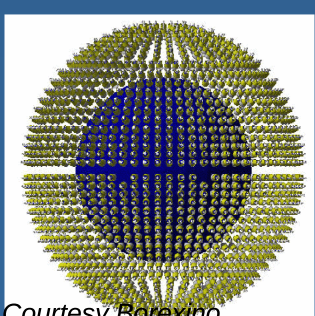


Courtesy H. Araujo and A. Howard, IC London


Courtesy GATE Collaboration


Courtesy R. Nartallo et al.,ESA

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


Courtesy Borexino

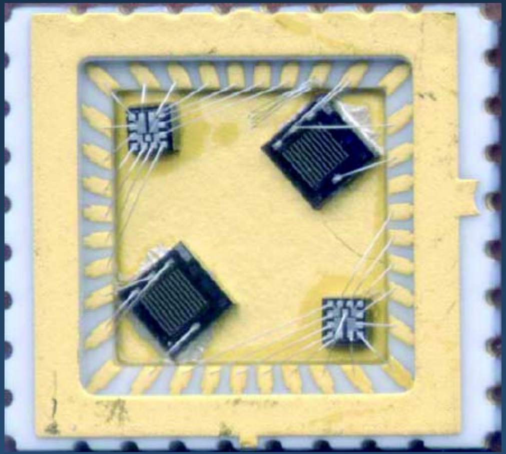
INFN Genova

Multi-disciplinary application environment

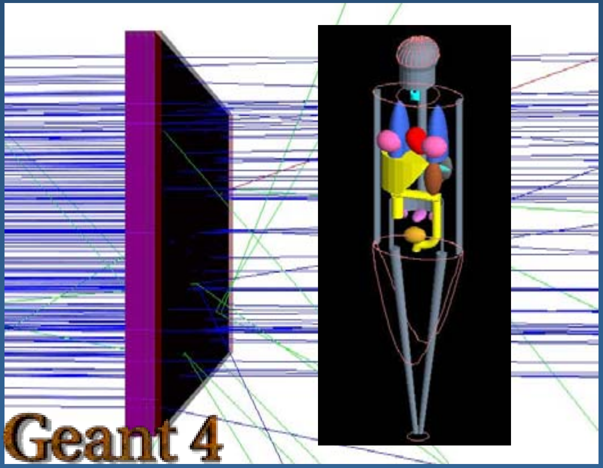
Space science

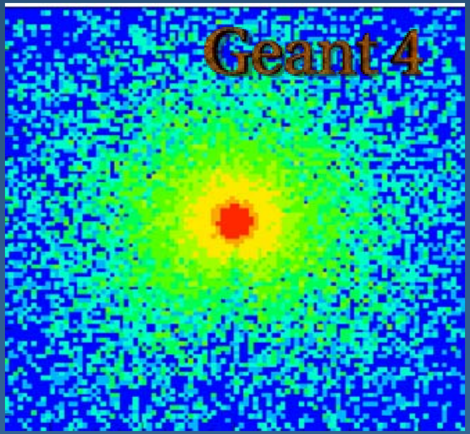
Dosimetry

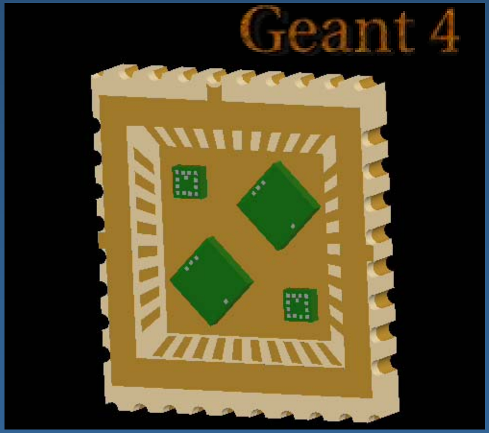
Radiotherapy



Effects on components



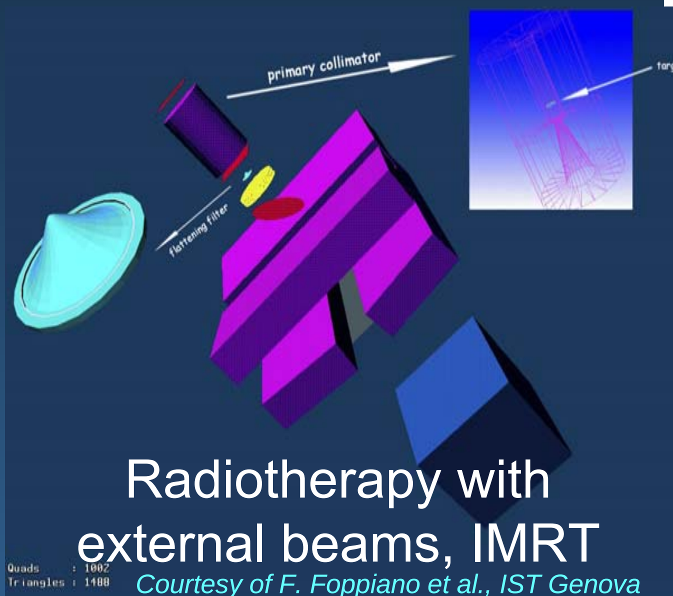


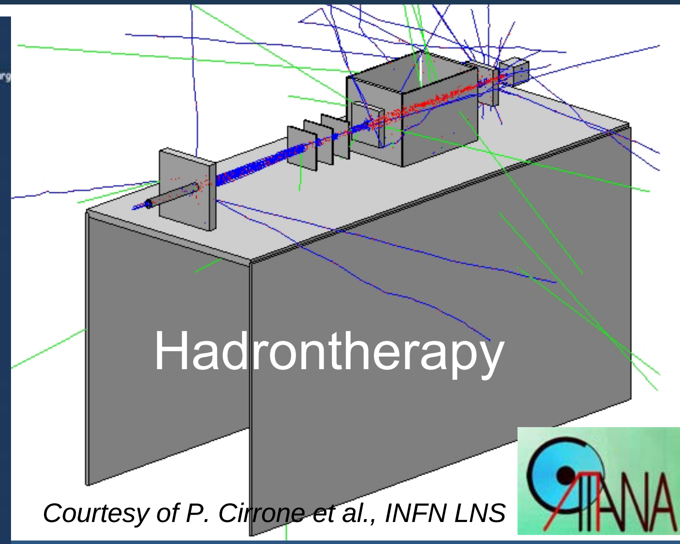


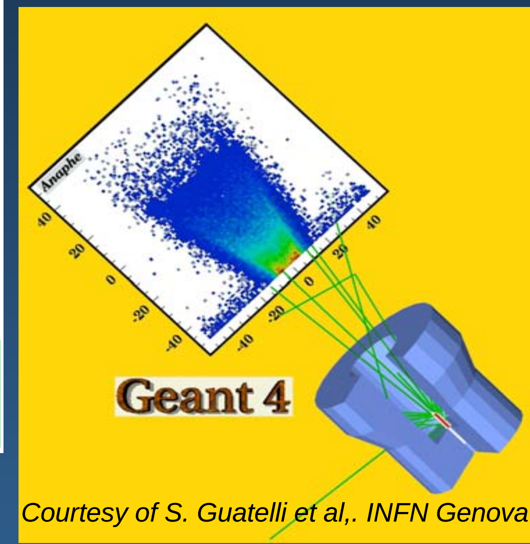
Wide spectrum of physics coverage, variety of physics models
Precise, quantitatively validated physics
Accurate description of geometry and materials

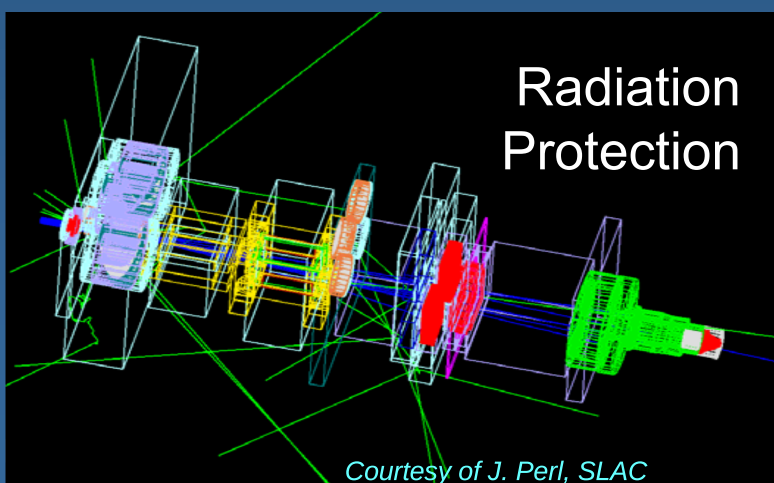
Geant 4

Dosimetry in Medical Applications

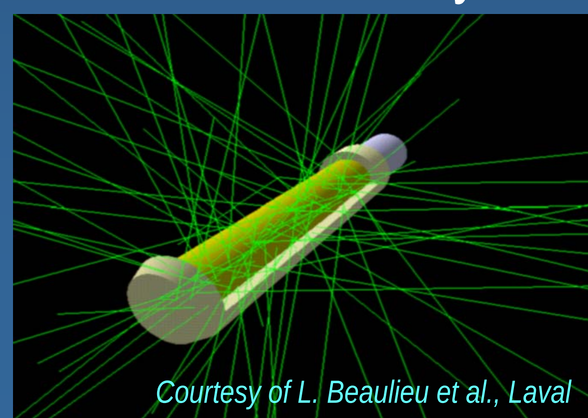








Brachytherapy



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

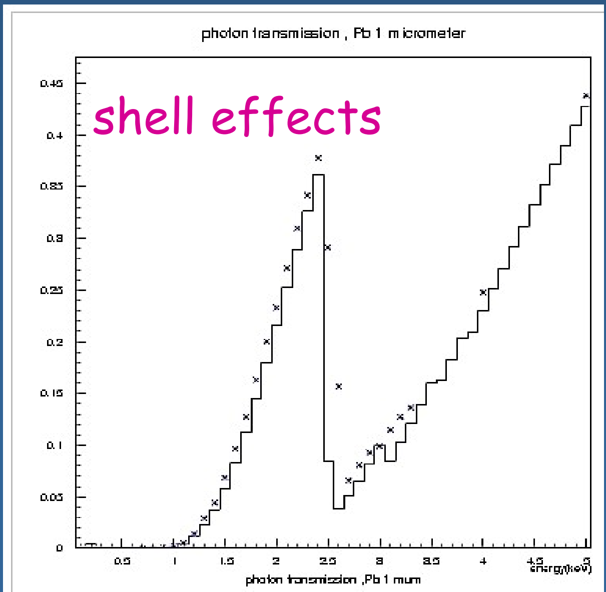
K. Manai, K. Farah, A.Trabelsi, F. Gharbi and O. Kadri (Tunisia)

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

Precise dose calculation

Geant4 Low Energy Electromagnetic Physics package

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



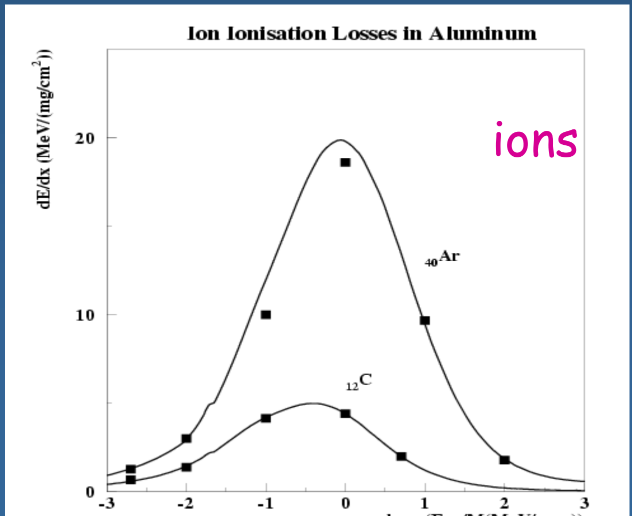
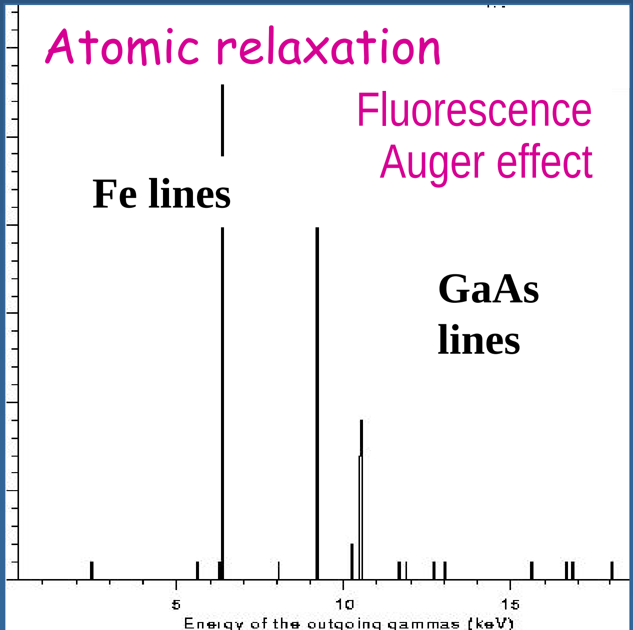
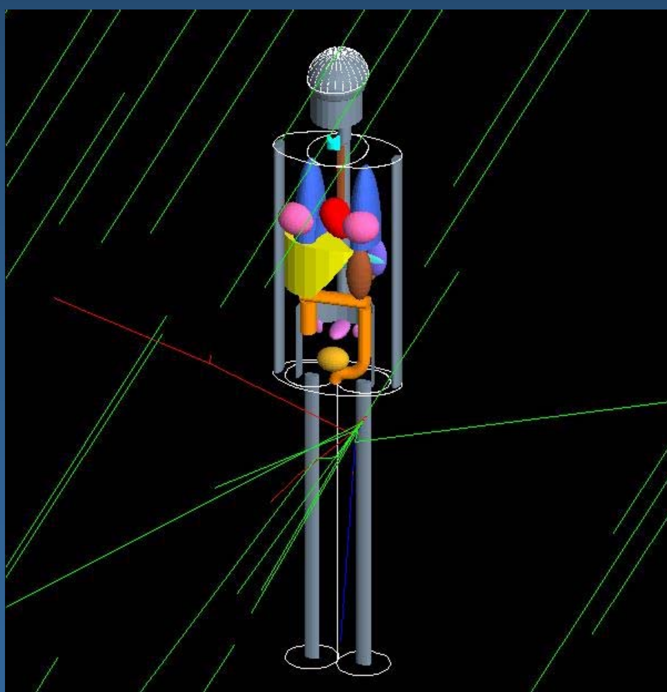


Figure 9: Ion electronic stopping power in aluminum. Points - the best fit on the data from Ref.[12], solid line - GEANT4 parameterisation. The accuracy of the data is about 5 %.



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

Geant 4
Anthropomorphic Phantoms



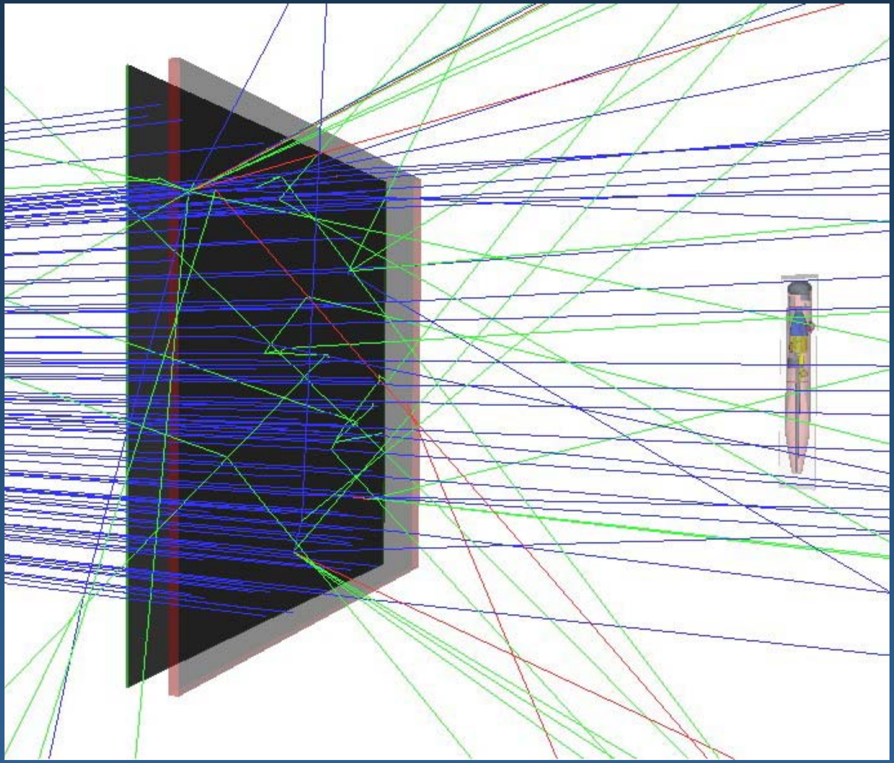
- Development of anthropomorphic phantom models for Geant4
  - evaluate dose deposited in critical organs
- Original approach
  - **analytical and voxel phantoms** in the same simulation environment

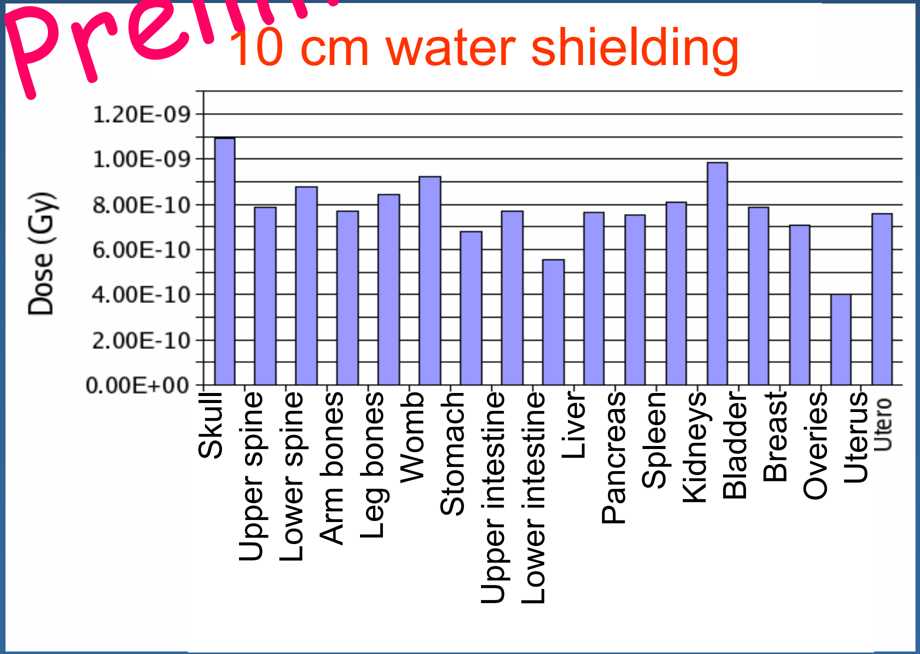
Analytical phantoms
Geant4 CSG, BREPS solids
Voxel phantoms
Geant4 parameterised volumes

GDML
for geometry description persistency

Maria Grazia Pia, *INFN Genova*

Radiation exposure of astronauts





Dose calculation in critical organs

Effects of external shielding
self-body shielding


Geant 4
DNA
2000/02/27 01:54
NRL
LASCO

Biological models in Geant4

Relevance for space: astronaut and aircrew radiation hazards

File Edit View Favorites Tools Help

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

Go Links

Geant 4 DNA

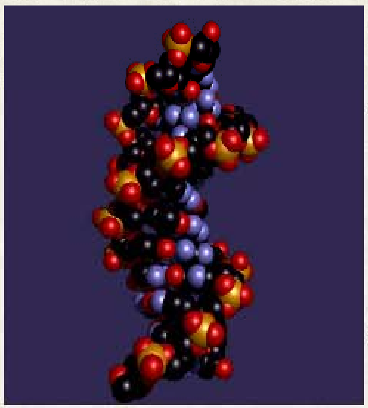
- Home

- 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

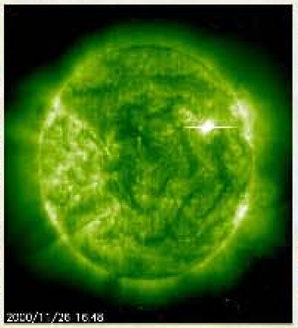


Estimating **cancer risk for human exposures to space radiation** is a challenge which involves a wide range of knowledge in physics, chemistry, biology and medicine.

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 DNA

ESA - INFN *(Genova)* - IN2P3 (*CENBG)*
New collaborators welcome!

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

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

Geant 4

Multiple domains in the same software environment

- Macroscopic level
  - calculation of dose
  - already feasible with Geant4
  - develop useful associated tools
- Cellular level
  - cell modelling
  - processes for cell survival, damage etc.
- DNA level
  - DNA modelling
  - physics processes at the eV scale
  - bio-chemical processes
  - processes for DNA damage, repair etc.

Complexity of

software, physics and biology

addressed with an iterative and incremental software process

↓

Parallel development at all the three levels

(domain decomposition)

Physics down to eV scale

- Complex domain
  - Physics: **collaboration with theorists**
  - Software: **innovative design** introduced in Geant4 (1st time in Monte Carlo)
- Many "track structure" Monte Carlo codes developed
  - Not publicly distributed
  - "Stand-alone" codes
- Geant4-DNA
  - Open source
  - "Track structure" simulation in a geenral-purpose Monte Carlo system

- Collaboration with experimentalists for model validation
  - Geant4 physics validation at low energies is difficult!

DNA level

New Low Energy Physics extensions

- Specialised processes down to eV scale
  - at this scale physics processes depend on material, phase etc.
- Models in liquid water
  - More realistic than water vapour
  - Theoretically more challenging
  - Hardly any experimental data
  - *New measurements needed (NPL?)*
- Status
  - 1st β-release Geant4 8.1
  - Improved design to be released in 2007
- Processes for other material than water
  - interest for radiation effects on components

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

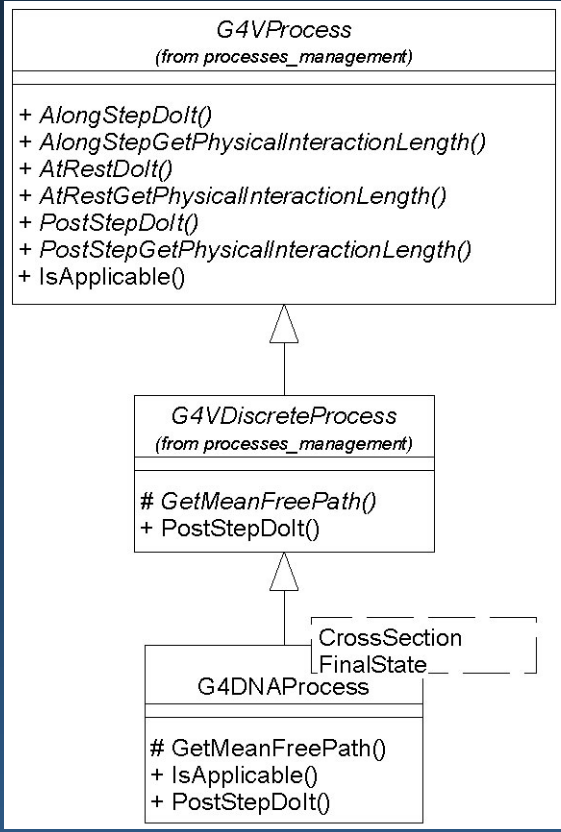
(Current) Physics Models

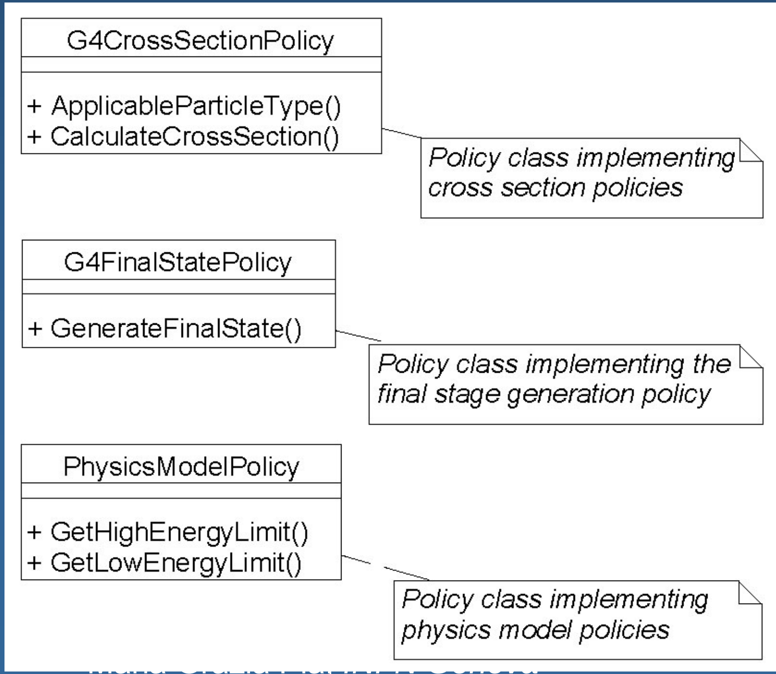
	e	p	H	α He+ He
Elastic	> 7.5 eV Screened Rutherford			
Excitation	7 eV – 10 keV A1B1, B1A1, Ryd A+B, Ryd C+D, diffuse bands	10 eV – 500 keV Dingfelder 300 keV – 10 MeV Emfietzoglou	100 eV – 10 MeV Dingfelder	Effective charge scaling from same models as for proton Dingfelder
Charge Change		100 eV – 10 MeV Dingfelder	100 eV – 10 MeV Dingfelder	
Ionisation	7 eV – 10 keV Emfietzoglou	100 eV – 500 keV Rudd 500 keV – 10 MeV Dingfelder (Born)	100 eV – 10 MeV Dingfelder	

What is behind…

Policy-based class design

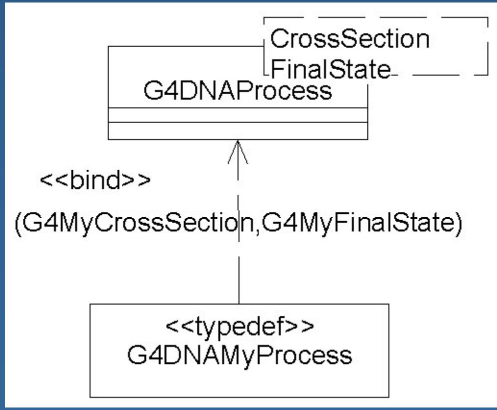
- A **policy** defines a class or class template **interface**
- **Policy host** classes are **parameterised** classes
  - *(classes that use other classes as a parameter)*
- Advantage w.r.t. a conventional strategy pattern:
  - Policies are not required to inherit from a base class
  - The code is **bound** at **compilation time**
    - No need of virtual methods, resulting in **faster** execution





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

More flexible design
Open to extension



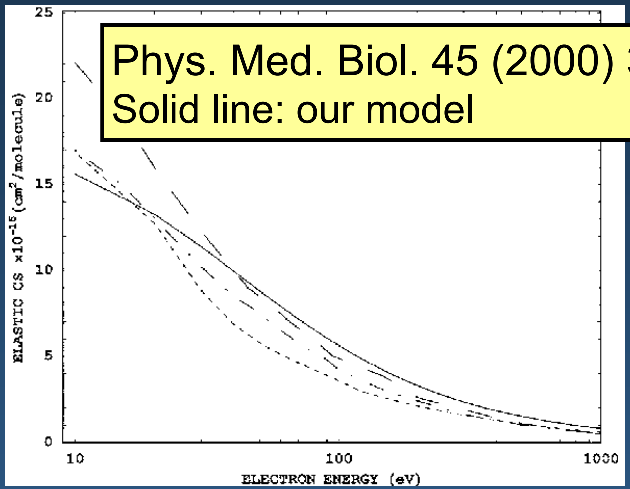
Why these models?

- No emotional attachment to any of the models
  - **Toolkit**: offer a wide choice among many available alternatives
  - Complementary models
  - No “one size fits all”
- Powerful design
  - Abstract interfaces: the kernel is blind to any specific modelling
  - Specialization of processes through template instantiation
  - Transparency of policy implementation
    - *e.g.: cross sections may be from analytical models or from experimental data*
  - Open proliferation of processes, policies and their instantiations
- Improvements, extensions, options
  - Open
  - Collaboration is welcome (experimental/modelling/software)
  - Sound software engineering

Elastic scattering

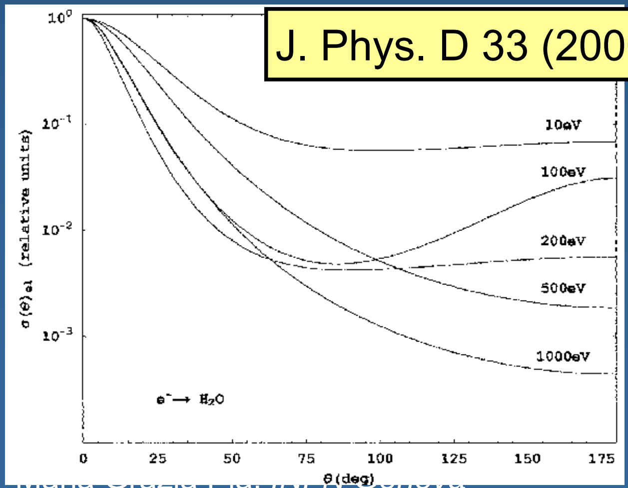
Total cross section

Phys. Med. Biol. 45 (2000) 3171-3194
Solid line: our model

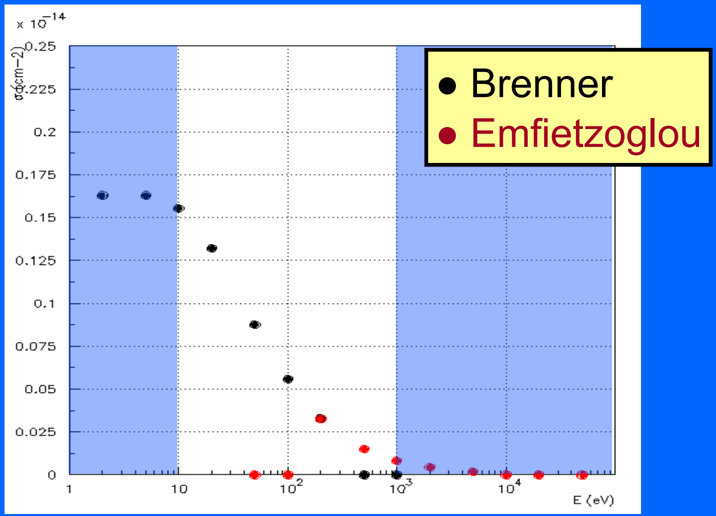


Angular distribution

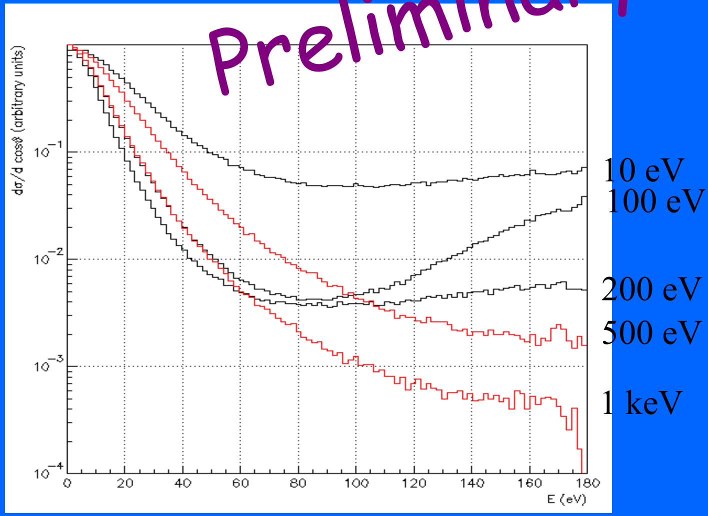
J. Phys. D 33 (2000) 932-944



Geant 4

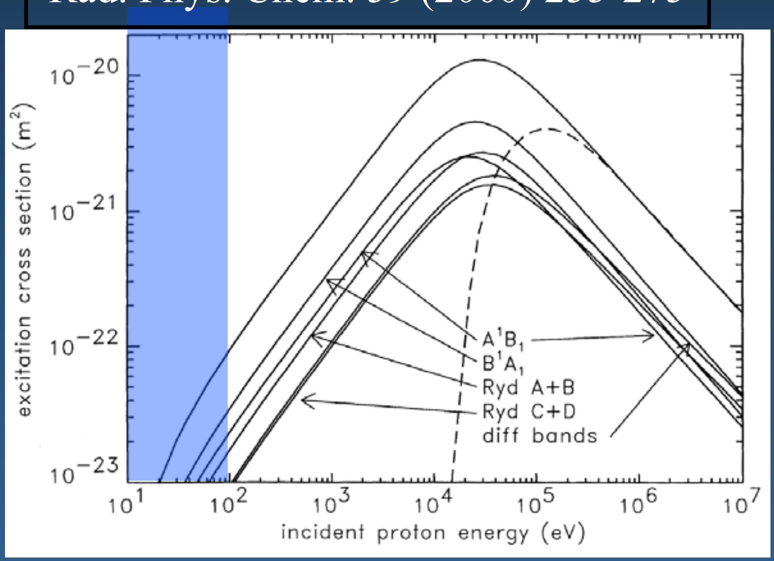


Preliminary

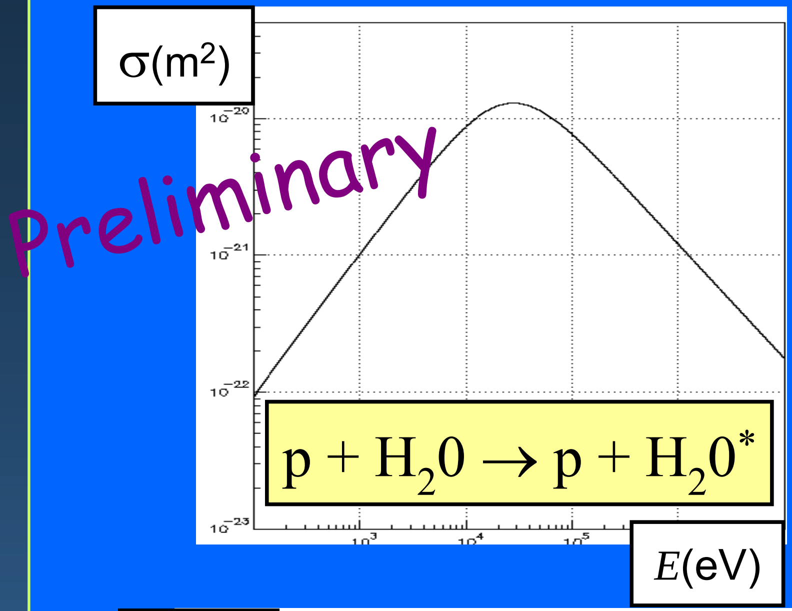


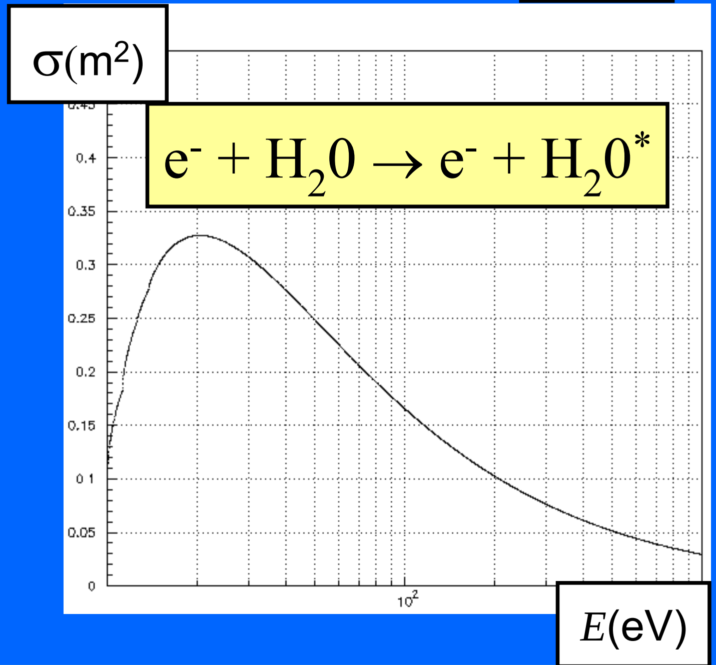
Excitation

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



Geant 4





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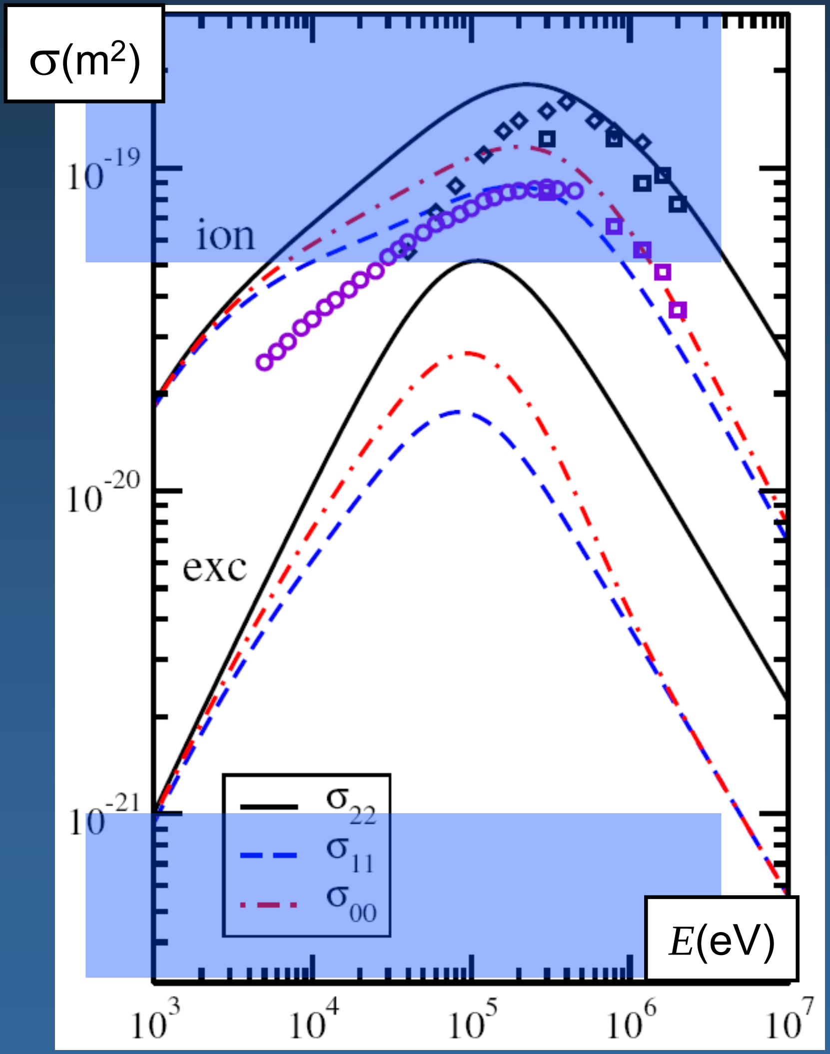
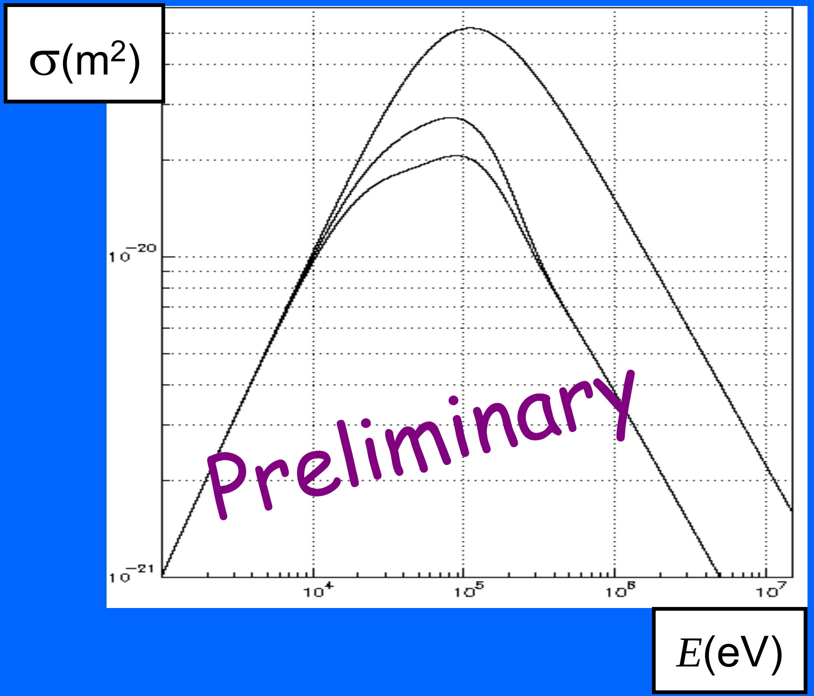
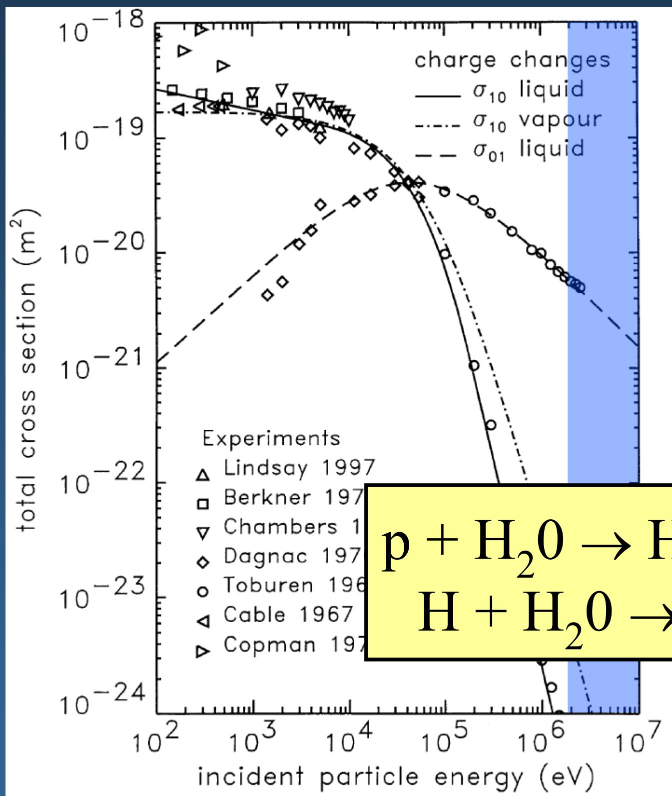


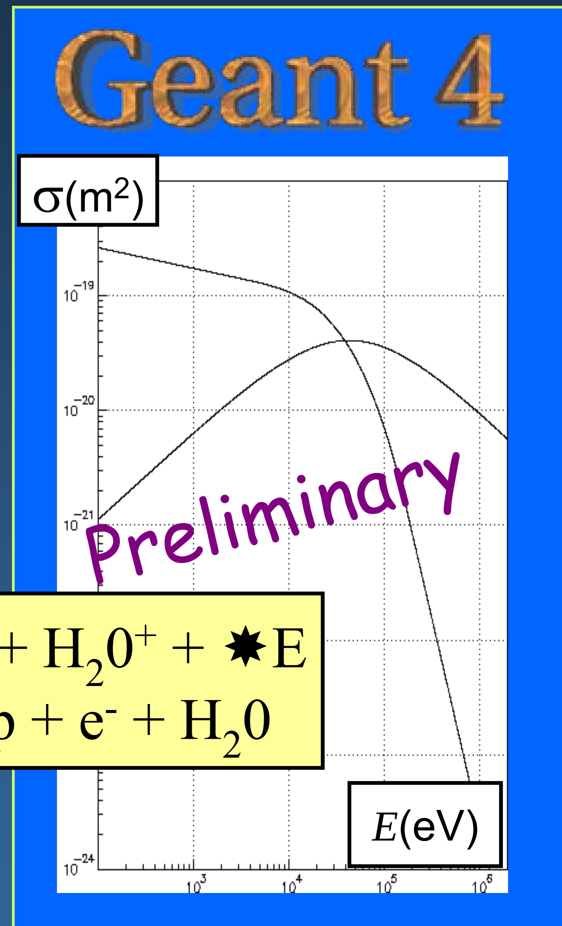
Geant 4

$$He + H_2O \rightarrow He + H_2O^*$$
$$He^+ + H_2O \rightarrow He^+ + H_2O^*$$
$$He^{++} + H_2O \rightarrow He^{++} + H_2O^*$$

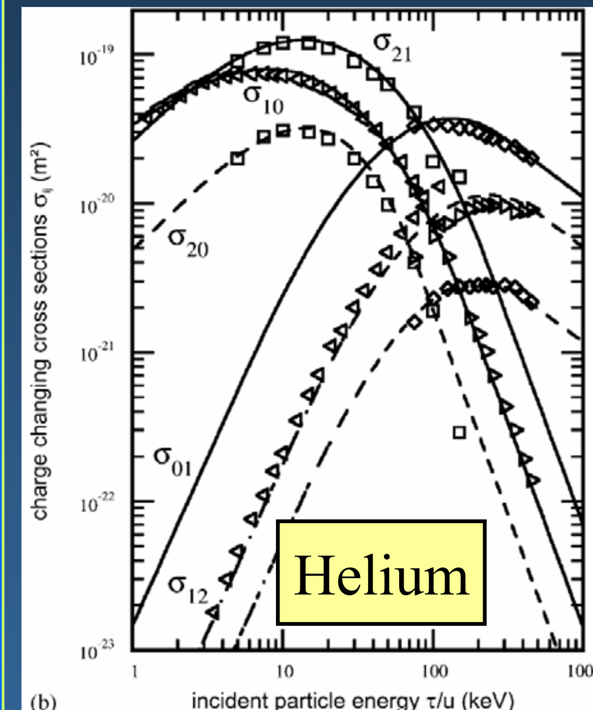


Charge transfer

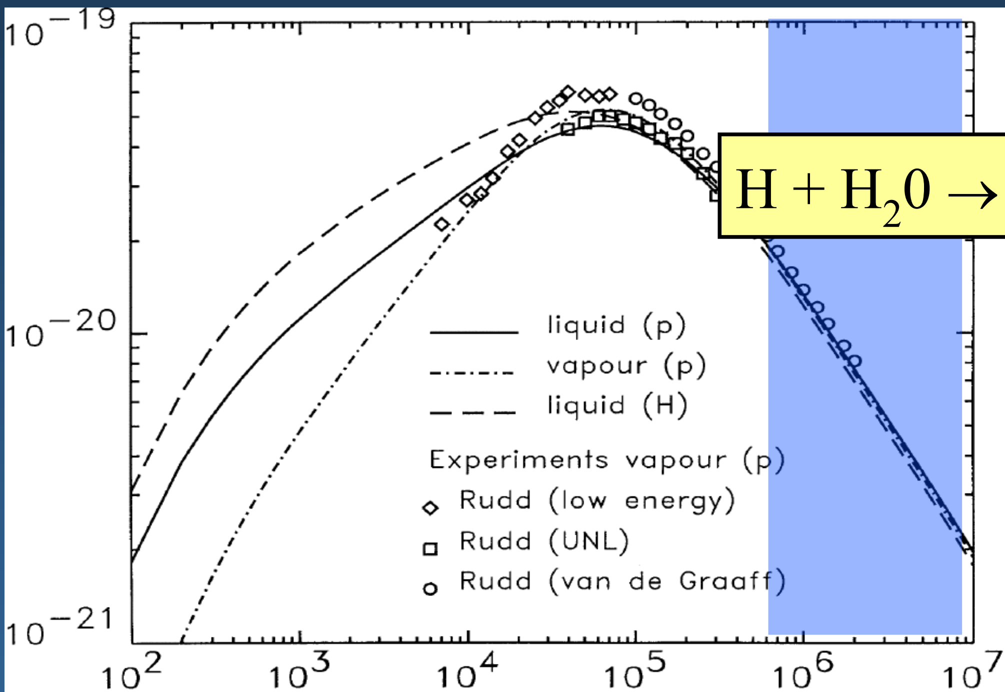


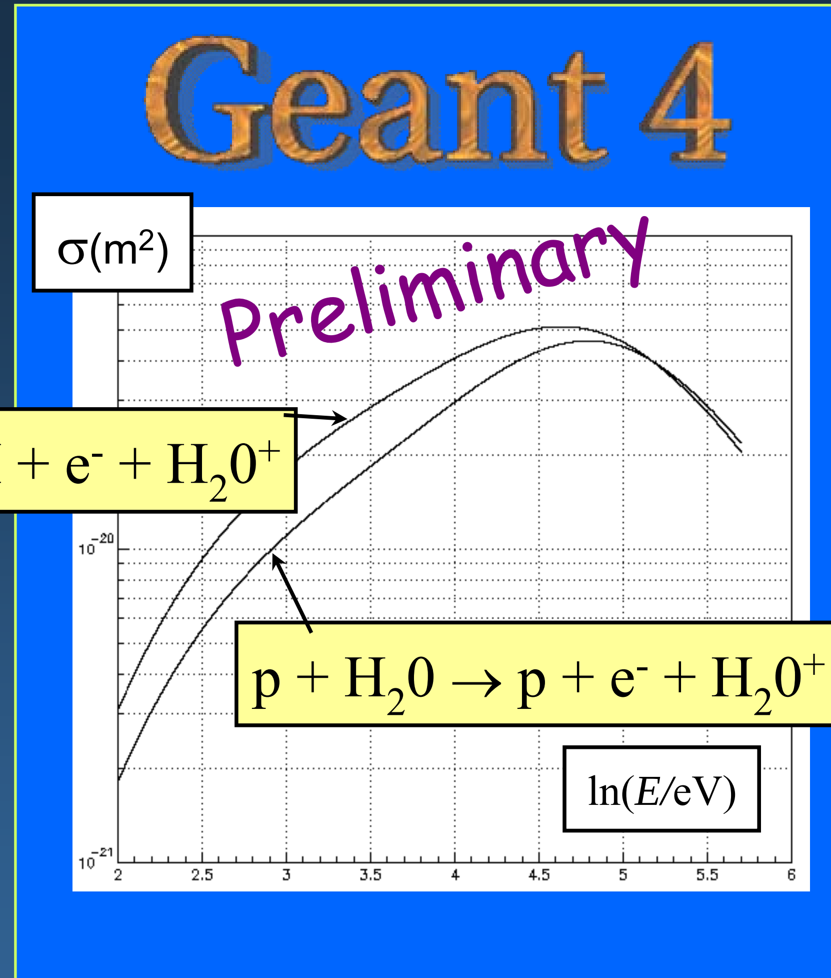


$$p + H_20 \rightarrow H + H_20^+ + ✸E$$
$$H + H_20 \rightarrow p + e^- + H_20$$

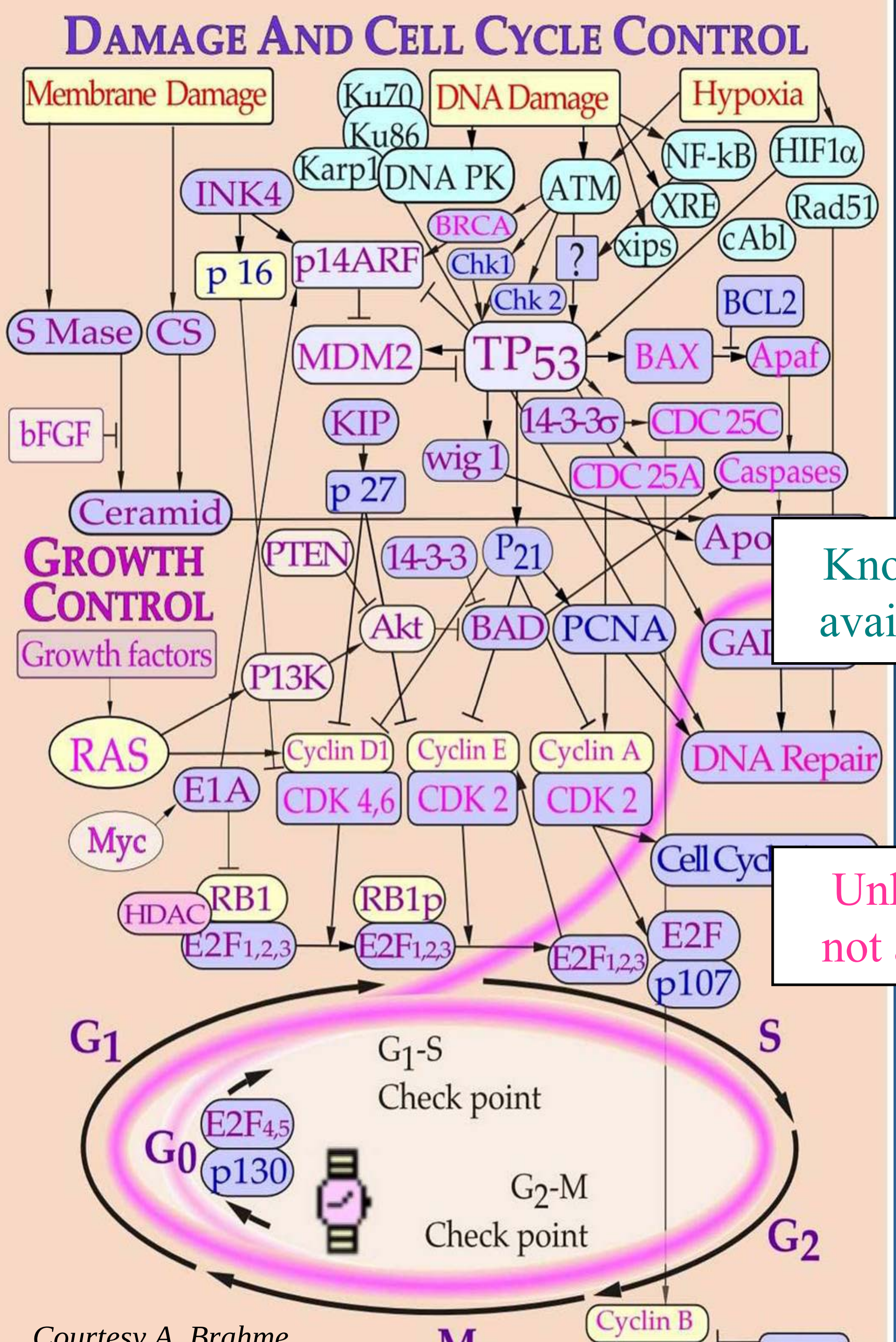


Ionisation

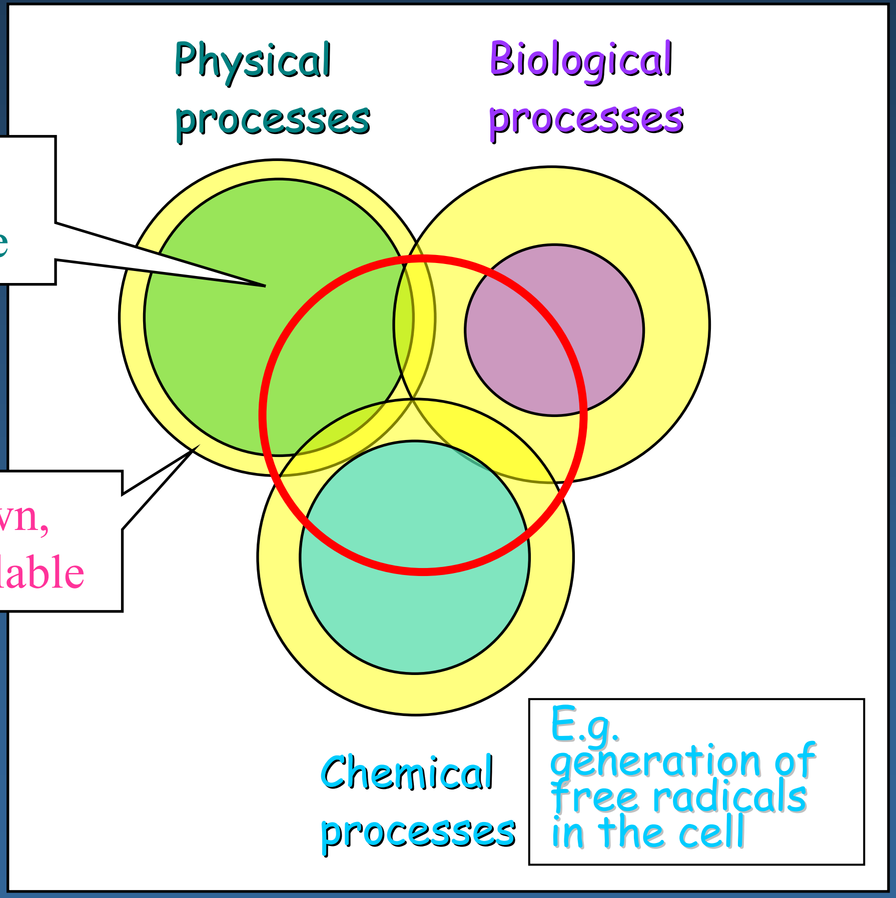

10^{-19}
10^{-20}
10^{-21}
10^2
10^3
10^4
10^5
10^6
10^7
liquid (p)
vapour (p)
liquid (H)
Experiments vapour (p)
Rudd (low energy)
Rudd (UNL)
Rudd (van de Graaff)


Geant 4
$\sigma(m^2)$
Preliminary
$H + H_20 \rightarrow H + e^- + H_20^+$
$p + H_20 \rightarrow p + e^- + H_20^+$
$\ln(E/eV)$
10^{-20}
10^{-21}
2
2.5
3
3.5
4
4.5
5
5.5
6

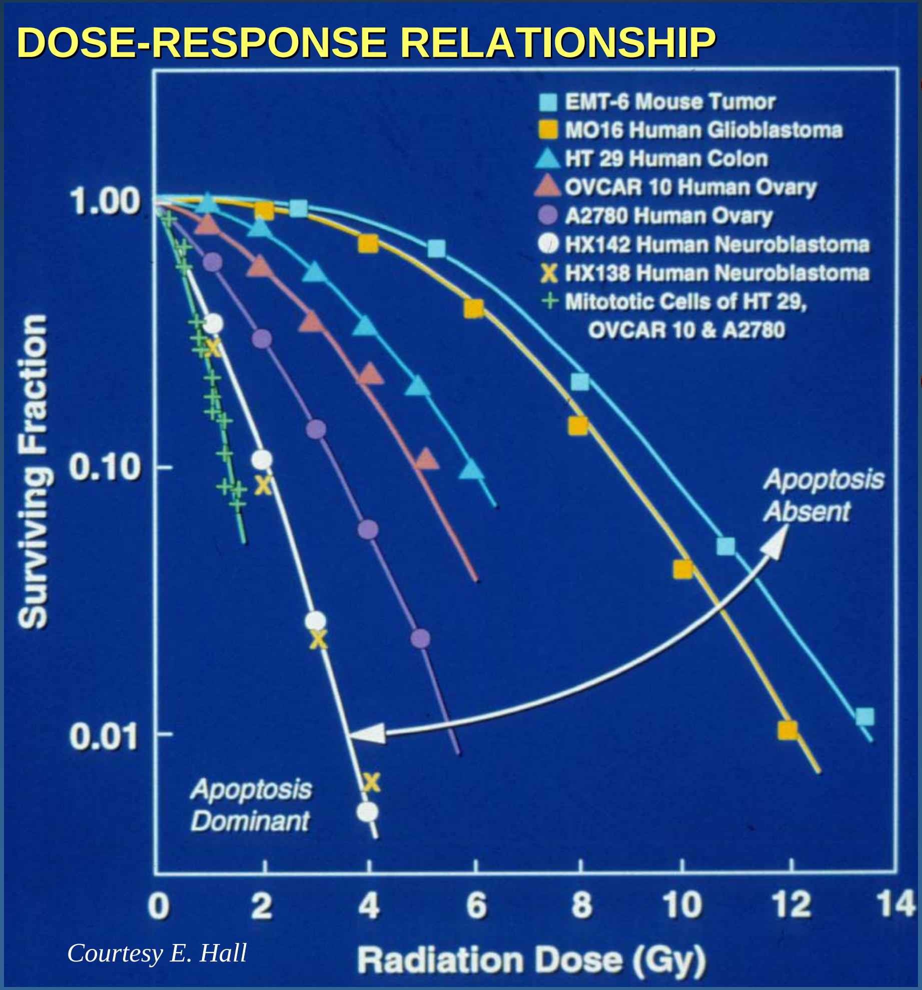
Biological processes



Courtesy A. Brahme (Karolinska Institute)



Biological effects: cell survival



Human cell lines irradiated with X-rays

- A cell survival curve describes the relationship between the **radiation dose** and the **proportion of cells that survive**
- Cell death
  - loss of the capacity for sustained proliferation or loss of reproductive integrity
  - A cell still may be *physically present* and *apparently intact*, but if it has lost the capacity to divide indefinitely and produce a large number of progeny, it is by definition dead

Theories and models for cell survival

TARGET THEORY MODELS
- Single-hit model
- Multi-target single-hit model
- Single-target multi-hit model

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

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

in progress

Geant 4

Requirements
Problem domain analysis

Analysis & Design
Implementation
Test

Incremental-iterative software process

Experimental validation of Geant4 simulation models

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

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

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

REVISED MODEL

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

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

In progress

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

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

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

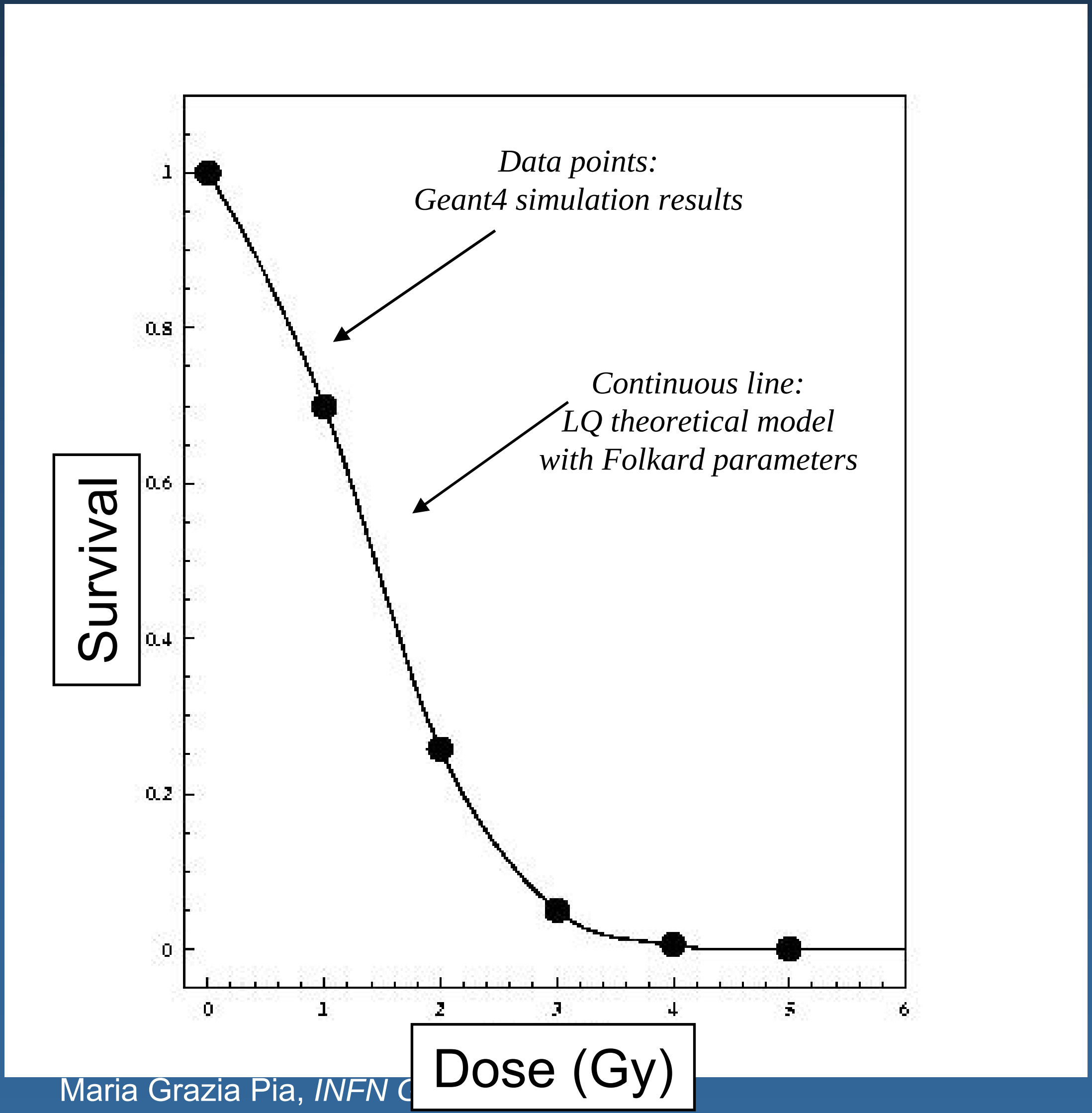
$$S = \exp\left[- N_{TOT}\left[1 + \frac{N_{PL}}{\varepsilon (1 - e^{-\varepsilon BAtr})}\right]^{\varepsilon} \right]$$

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

$$-\ln[S(t)] = (\eta_{AC} + \eta_{AB}) D - \varepsilon \ln[1 + (\eta_{AB} D/\varepsilon)(1 - e^{-\varepsilon BA\, tr})]$$

$$-\ln[S(t)] = (\eta_{AC} + \eta_{AB}\, e^{-\varepsilon BAtr}) D + (\eta^2_{AB}/2\varepsilon)(1 - e^{-\varepsilon BA\, tr})^2 D^2]$$

Cell survival models verification



Monolayer

V79-379A cells

Proton beam
E= 3.66 MeV/n

LQ model

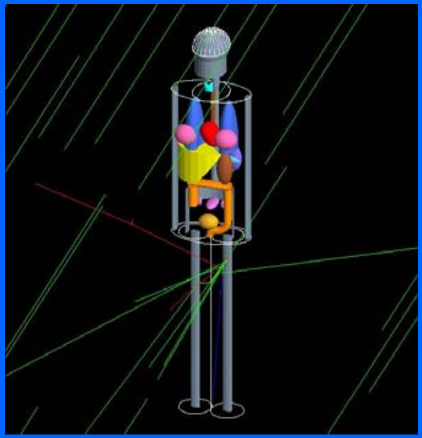
$$S = e^{-\alpha D - \beta D^2}$$

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

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

Scenario
for Mars (and earth…)

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



Dose in
organs at risk

Phase space input
to nano-simulation

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

Oncological risk to
astronauts/patients

Risk of nervous
system damage

Geant4 simulation with
physics at eV scale
+
DNA processes

Geant 4

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

Wide spectrum of complementary and alternative physics models

Multi-disciplinary dosimetry simulation

Precision of physics
Versatility of experimental modelling

Geant 4 DNA

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

Multiple levels in the same simulation environment

Conventional dosimetry
Models at cellular level
Models at DNA level

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