Geant4 for Microdosimetry

Maria Grazia Pia
INFN Genova, Italy

on behalf of the Geant4-DNA Team
S. Chauvie, Z. Francis, S. Guatelli, S. Incerti, B. Mascialino, Ph. Moretto, G. Montarou, P. Nieminen

RADAM06
Groningen, 6-9 June 2006
Object Oriented Toolkit
for the simulation of particle interactions with matter

also...

An experiment of
distributed software production and management

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

1st release: December 1998
2 new releases/year since then

http://cern.ch/geant4
http://www.ge.infn.it/geant4
Geant 4

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
- Pest control, food irradiation
- Humanitarian projects, security
- etc.
- Technology transfer to industry, hospitals...

Most cited “engineering” publication in the past 2 years!
Geant4 architecture

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

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

- Physics independent from tracking

- Subject to rigorous, quantitative validation

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

- Hadronic physics
  - Parameterised, data-/theory-driven models

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

Domain decomposition

Hierarchical structure of sub-domains

Uni-directional flow of dependencies

Interface to external products w/o dependencies
Geant4 Collaboration

~100 members

MoU based
Development, Distribution and User Support of Geant4

Major physics laboratories:
CERN, KEK, SLAC, TRIUMF, TJNL

European Space Agency:
ESA

National Institutes:
INFN, IN2P3, PPARC

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

Maria Grazia Pia, INFN Genova
Multi-disciplinary application environment

Dosimetry

- Space science
- Radiotherapy
- Effects on components

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

Maria Grazia Pia, INFN Genova
Dosimetry in Medical Applications

Geant 4

Radiotherapy with external beams, IMRT
Courtesy of F. Foppiano et al., IST Genova

Hadrontherapy
Courtesy of P. Cirrone et al., INFN LNS

Brachytherapy
Courtesy of L. Beaulieu et al., Laval

Radiation Protection
Courtesy of J. Perl, SLAC

Courtesy of S. Guatelli et al., INFN Genova

Courtesy of J. Perl, SLAC
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

![Graphs of photon interaction, ionization losses, and atomic relaxation](image.png)
Medical LINAC for IMRT

Accuracy

**Depth dose profile**

Simulated data vs experimental data match perfectly, with a **p-value = 1**.

**Lateral dose profile**

- **Simulation vs experimental data**
  - Tissue vs tumor distinction is clearly visible.

**Kolmogorov-Smirnov test**

<table>
<thead>
<tr>
<th>Range</th>
<th>D</th>
<th>p-value</th>
</tr>
</thead>
<tbody>
<tr>
<td>-84 ÷ -60 mm</td>
<td>0.385</td>
<td>0.23</td>
</tr>
<tr>
<td>-59 ÷ -48 mm</td>
<td>0.27</td>
<td>0.90</td>
</tr>
<tr>
<td>-47 ÷ 47 mm</td>
<td>0.43</td>
<td>0.19</td>
</tr>
<tr>
<td>48 ÷ 59 mm</td>
<td>0.30</td>
<td>0.82</td>
</tr>
<tr>
<td>60 ÷ 84 mm</td>
<td>0.40</td>
<td>0.10</td>
</tr>
</tbody>
</table>
**Flexibility**

Endocavitary brachytherapy

- MicroSelectron-HDR source

Interstitial brachytherapy

- Bebig Isoseed I-125 source

Superficial brachytherapy

- Geant 4
**Dosimetry: protons and ions**

<table>
<thead>
<tr>
<th>Goodness of Fit</th>
<th>Cramer – von Mises test</th>
<th>Anderson – Darling test</th>
</tr>
</thead>
<tbody>
<tr>
<td>Test statistics</td>
<td>0.06</td>
<td>0.499375</td>
</tr>
<tr>
<td>p-value</td>
<td>0.79</td>
<td>0.747452</td>
</tr>
</tbody>
</table>

**Electromagnetic only**

| CHIPS        | 0.52 | 0.443831 |

**Inventory of Geant4 hadronic models**

- CHIPS (gamma)
- Photo-nuclear, electro-nuclear
- FTF String (up to 20 TeV)
- QG String (up to 100 TeV)
- Binary cascade
- LE pp, pn
- HEP (up to 20 TeV)
- LEP

Further validation tests in progress.
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

Maria Grazia Pia, INFN Genova
Radiation protection for interplanetary manned missions

- Galactic and extra-galactic cosmic rays
- Neutrinos
- Solar X-rays
- Secondary emissions
- Trapped particles
- Solar flare neutrons and γ-rays
- Anomalous cosmic rays
- Jovian electrons
- Solar event protons, electrons, and heavy ions
S. Guatelli et al., Geant4 Simulation for interplanetary manned missions

Doubling the shielding thickness decreases the energy deposit by ~10%
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
Radiation exposure of astronauts

Dose calculation in critical organs

Effects of external shielding
self-body shielding

Maria Grazia Pia, INFN Genova
Processes are handled transparently by Geant4 kernel through an abstract interface.

Geometry objects (solids, logical volumes, physical volumes) are handled transparently by Geant4 kernel through abstract interfaces.

So why not describing DNA?

So what about mutagenesis as a process?
Biological models in Geant4

Relevance for space: astronaut and aircrew radiation hazards
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.
Simulation of nano-scale effects of radiation at the DNA level

- Various scientific domains involved
  - medical, biology, genetics, physics, software engineering
- Multiple approaches can be implemented with Geant4
  - RBE parameterisation, detailed biochemical processes, etc.

First phase: 2000-2001
- Collection of user requirements & first prototypes

Second phase: started in 2004
- Software development & open source release
Physics

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

“It was noted that experiments have requirements for independent, alternative physics models. In Geant4 these models, differently from the concept of packages, allow the user to understand how the results are produced, and hence improve the physics validation. Geant4 is developed with a modular architecture and is the ideal framework where existing components are integrated and new models continue to be developed.”
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

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

OO technology

Strategic vision

Toolkit
Biological processes

- Known, available
  - E.g. generation of free radicals in the cell
- Physical processes
- Biological processes
- Chemical processes

Known, available

Unknown, not available
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)

Maria Grazia Pia, INFN Genova
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

- **Analysis & Design Implementation Test**

- **Experimental validation of Geant4 simulation models**

- **Requirements Problem domain analysis**

Maria Grazia Pia, INFN Genova
<table>
<thead>
<tr>
<th>TARGET THEORY</th>
<th>SINGLE-HIT THEORY</th>
</tr>
</thead>
<tbody>
<tr>
<td>TARGET THEORY</td>
<td>MULTI-TARGET</td>
</tr>
<tr>
<td>MOLECULAR THEORY</td>
<td>RADIATION ACTION</td>
</tr>
<tr>
<td>MOLECULAR THEORY</td>
<td>DUAL RADIATION ACTION</td>
</tr>
<tr>
<td>MOLECULAR THEORY</td>
<td>REPAIR-MISREPAIR LIN REP / QUADMIS</td>
</tr>
<tr>
<td>MOLECULAR THEORY</td>
<td>REPAIR-MISREPAIR LIN REP / MIS</td>
</tr>
<tr>
<td>MOLECULAR THEORY</td>
<td>LETHAL-POTENTIALLY LETHAL</td>
</tr>
<tr>
<td>MOLECULAR THEORY</td>
<td>LETHAL-POTENTIALLY LETHAL – LOW DOSE</td>
</tr>
<tr>
<td>MOLECULAR THEORY</td>
<td>LETHAL-POTENTIALLY LETHAL – HIGH DOSE</td>
</tr>
<tr>
<td>MOLECULAR THEORY</td>
<td>LETHAL-POTENTIALLY LETHAL – LQ APPROX</td>
</tr>
</tbody>
</table>

**REVISED MODEL**

\[ S = e^{-\frac{D}{D_0}} \]

\[ S = 1 - (1 - e^{-qD})^n \]

\[ S = e^{-q_1D} \left[ 1 - (1 - e^{-q_2D})^n \right] \]

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

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

\[ S = e^{-\alpha D\left[1 + (\alpha DT / \varepsilon)\right]^{\varepsilon}} \]

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

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

\[ S = e^{-\eta_{AC} D} \]

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

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

Maria Grazia Pia, *INFN Genova*
Low Energy Physics extensions

- Specialised processes down to the eV scale
  - at this scale physics processes depend on material, phase etc.
  - in progress: Geant4 processes in water at the eV scale
  - β-release: Friday 30 June 2006

- Processes for other material than water to follow
  - interest for radiation effects on components

Current status

<table>
<thead>
<tr>
<th></th>
<th>Electrons</th>
<th>Protons (H+)</th>
<th>Hydrogen (H)</th>
<th>Alpha (He++)</th>
<th>He+</th>
<th>He</th>
</tr>
</thead>
<tbody>
<tr>
<td>Elastic</td>
<td>Brenner (7.5 - 200 eV)</td>
<td>Negligible effect</td>
<td>Negligible effect</td>
<td>Negligible effect</td>
<td>Negligible effect</td>
<td>Negligible effect</td>
</tr>
<tr>
<td></td>
<td>Emfietzoglou (&gt; 200 ev)</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Excitation</td>
<td>Born (7 eV – 10 keV)</td>
<td>Negligible effect</td>
<td>Miller and Green (100 eV – 10 MeV)</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>Born (100 eV – 10 MeV)</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Charge decrease</td>
<td>Not pertinent to this particle</td>
<td>Dingfelder (100 eV – 2 MeV)</td>
<td>Not pertinent to this particle</td>
<td>In progress</td>
<td>In progress</td>
<td>Not pertinent to this particle</td>
</tr>
<tr>
<td>Charge increase</td>
<td>Not pertinent to this particle</td>
<td>Not pertinent to this particle</td>
<td>Miller and Green</td>
<td>Not pertinent to this particle</td>
<td>In progress</td>
<td>In progress</td>
</tr>
<tr>
<td></td>
<td>Rudd (0.1 - 500 keV)</td>
<td>In progress (&gt; 500 keV)</td>
<td>Rudd (0.1 – 100 MeV)</td>
<td>In progress</td>
<td>In progress</td>
<td>In progress</td>
</tr>
</tbody>
</table>

Maria Grazia Pia, INFN Genova
Development process

- Complex domain
  - physics
  - software

- Collaboration with theorists

- Innovative design introduced in Geant4
  - Policy-based class design
  - Parameterised classes: policies are cross section models, models for final state calculation etc.
  - Flexibility of modelling + performance optimisation

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

<table>
<thead>
<tr>
<th></th>
<th>Electrons</th>
<th>Protons (H+)</th>
<th>Hydrogen (H)</th>
<th>Alpha (He++)</th>
<th>He+</th>
<th>He</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Elastic</strong></td>
<td>Brenner (7.5 - 200 eV)</td>
<td>Negligible effect</td>
<td>Negligible effect</td>
<td>Negligible effect</td>
<td>Negligible effect</td>
<td>Negligible effect</td>
</tr>
<tr>
<td></td>
<td>Emfietzoglou (&gt; 200 eV)</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td><strong>Excitation</strong></td>
<td>Emfietzoglou</td>
<td>Miller and Green</td>
<td>Negligible effect</td>
<td>Miller and Green</td>
<td>Miller and Green</td>
<td>Miller and Green</td>
</tr>
<tr>
<td></td>
<td>Born (100 eV – 10 MeV)</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td><strong>Charge decrease</strong></td>
<td>Process not pertinent to this particle</td>
<td>Process not pertinent to this particle</td>
<td>Miller and Green</td>
<td>Miller and Green</td>
<td>Miller and Green</td>
<td>Miller and Green</td>
</tr>
<tr>
<td></td>
<td>Dingfelder</td>
<td>(100 eV – 2 MeV)</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td><strong>Charge increase</strong></td>
<td>Process not pertinent to this particle</td>
<td>Process not pertinent to this particle</td>
<td>Miller and Green</td>
<td>Miller and Green</td>
<td>Miller and Green</td>
<td>Miller and Green</td>
</tr>
<tr>
<td></td>
<td>Dingfelder</td>
<td>(0.1 Kev – 100 MeV)</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td><strong>Ionization</strong></td>
<td>In progress</td>
<td>Rudder (0.1 - 500 keV)</td>
<td>In progress (&gt; 500 keV)</td>
<td>Rudder (0.1 – 100 MeV)</td>
<td>In progress</td>
<td>In progress</td>
</tr>
</tbody>
</table>

### Process kinematics

<table>
<thead>
<tr>
<th></th>
<th>Electrons</th>
<th>Protons (H+)</th>
<th>Hydrogen (H)</th>
<th>Alpha (He++)</th>
<th>He+</th>
<th>He</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Elastic</strong></td>
<td>Brenner (7.5 - 200 eV)</td>
<td>Negligible effect</td>
<td>Negligible effect</td>
<td>Negligible effect</td>
<td>Negligible effect</td>
<td>Negligible effect</td>
</tr>
<tr>
<td></td>
<td>Emfietzoglou (&gt; 200 eV)</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td><strong>Excitation</strong></td>
<td>Emfietzoglou</td>
<td>Miller and Green</td>
<td>Negligible effect</td>
<td>Miller and Green</td>
<td>Miller and Green</td>
<td>Miller and Green</td>
</tr>
<tr>
<td></td>
<td>Born (100 eV – 10 MeV)</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td><strong>Charge decrease</strong></td>
<td>Process not pertinent to this particle</td>
<td>Process not pertinent to this particle</td>
<td>Miller and Green</td>
<td>Miller and Green</td>
<td>Miller and Green</td>
<td>Miller and Green</td>
</tr>
<tr>
<td></td>
<td>Dingfelder</td>
<td>(100 eV – 2 MeV)</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td><strong>Charge increase</strong></td>
<td>Process not pertinent to this particle</td>
<td>Process not pertinent to this particle</td>
<td>Miller and Green</td>
<td>Miller and Green</td>
<td>Miller and Green</td>
<td>Miller and Green</td>
</tr>
<tr>
<td></td>
<td>Dingfelder</td>
<td>(0.1 Kev – 100 MeV)</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td><strong>Ionization</strong></td>
<td>In progress</td>
<td>Rudder (0.1 - 500 keV)</td>
<td>In progress (&gt; 500 keV)</td>
<td>Rudder (0.1 – 100 MeV)</td>
<td>In progress</td>
<td>In progress</td>
</tr>
</tbody>
</table>

### Final state generation

<table>
<thead>
<tr>
<th></th>
<th>Electrons</th>
<th>Protons (H+)</th>
<th>Hydrogen (H)</th>
<th>Alpha (He++)</th>
<th>He+</th>
<th>He</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Elastic</strong></td>
<td>Brenner (7.5 - 200 eV)</td>
<td>Negligible effect</td>
<td>Negligible effect</td>
<td>Negligible effect</td>
<td>Negligible effect</td>
<td>Negligible effect</td>
</tr>
<tr>
<td></td>
<td>Emfietzoglou (&gt; 200 eV)</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td><strong>Excitation</strong></td>
<td>Emfietzoglou</td>
<td>Miller and Green</td>
<td>Negligible effect</td>
<td>Miller and Green</td>
<td>Miller and Green</td>
<td>Miller and Green</td>
</tr>
<tr>
<td></td>
<td>Born (100 eV – 10 MeV)</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td><strong>Charge decrease</strong></td>
<td>Process not pertinent to this particle</td>
<td>Process not pertinent to this particle</td>
<td>Miller and Green</td>
<td>Miller and Green</td>
<td>Miller and Green</td>
<td>Miller and Green</td>
</tr>
<tr>
<td></td>
<td>Dingfelder</td>
<td>(100 eV – 2 MeV)</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td><strong>Charge increase</strong></td>
<td>Process not pertinent to this particle</td>
<td>Process not pertinent to this particle</td>
<td>Miller and Green</td>
<td>Miller and Green</td>
<td>Miller and Green</td>
<td>Miller and Green</td>
</tr>
<tr>
<td></td>
<td>Dingfelder</td>
<td>(0.1 Kev – 100 MeV)</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td><strong>Ionization</strong></td>
<td>In progress</td>
<td>Rudder (0.1 - 500 keV)</td>
<td>In progress (&gt; 500 keV)</td>
<td>Rudder (0.1 – 100 MeV)</td>
<td>In progress</td>
<td>In progress</td>
</tr>
</tbody>
</table>
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


Solid line: our model

Angular distribution


Preliminary
Excitation


Maria Grazia Pia, INFN Genova

\[
p + H_2O \rightarrow p + H_2O^* \\
\]

\[
e^- + H_2O \rightarrow e^- + H_2O^* \\
\]

\[\sigma(m^2)\]

\[E(eV)\]

\[E(eV)\]
Excitation

He + H₂O → He + H₂O*
He⁺ + H₂O → He⁺ + H₂O*
He++ + H₂O → He++ + H₂O*

σ(m²)


Preliminary
Charge transfer

\[ p + H_2O \rightarrow H + H_2O^+ + 1E \]
\[ H + H_2O \rightarrow p + e^- + H_2O \]

Helium

Preliminary

E(eV)

σ(m²)

incident particle energy (eV)

incident particle energy (keV)

Maria Grazia Pia, INFN Genova
Ionisation

$\ln\left(\frac{E}{\text{eV}}\right)$

$\sigma(\text{m}^2)$

$H + H_2O \rightarrow H + e^- + H_2O^+$

$p + H_2O \rightarrow p + e^- + H_2O^+$

Maria Grazia Pia, INFN Genova
What is behind...

Elastic scattering

Maria Grazia Pia, INFN Genova
...and more

**Excitation**

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

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

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

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

The code is **bound** at **compilation time**

No need of virtual methods, resulting in **faster** execution

---

**Rigorous software engineering**

Sophisticated design based on advanced **technology**

Maria Grazia Pia, *INFN Genova*
...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

Maria Grazia Pia, INFN Genova
**Distributed computing environment**

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

---

**DIANE**

Distributed Analysis Environment

Developed by J. Moscicki, CERN/IT

http://cern.ch/DIANE

---

**Master-Worker**

architectural pattern

---

**Parallel cluster processing**

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

---

Maria Grazia Pia, INFN Genova
UML Deployment Diagram

Transparent to the user:

same Geant4 application code in sequential and parallel execution mode

Results presented at CHEP06
Publication in preparation

Maria Grazia Pia, INFN Genova
Traceback from a run on grid testbed

Current #Grid setup (computing elements):

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

**Multiple levels**
**in the same simulation environment**

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

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

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

What is the impact of what we are doing?

Software ➔ Knowledge made usable

Proposal

Joint Geant4-DNA / COST Workshop

Common concrete objectives
Collaborative projects

Feedback
Improvement
Extension

- Experimental measurements
- Theoretical models
- Software

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

Maria Grazia Pia, INFN Genova