Design and performance evaluation of
generic programming techniques
in a R&D prototype of Geant4 physics

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Acknowledgments

The physics models and original implementations of the physics processes mentioned in this talk derive from Geant4 Standard and Low Energy Electromagnetic packages as in Geant4 9.1-9.2

Thanks to

- **Sergio Bertolucci** (INFN and CERN)
- **Tom Evans** (ORNL)
- **Simone Giani** (CERN)
- **Alessandro Montanari** (INFN Bologna)
- **Andreas Pfeiffer** (CERN)

for helpful discussions and advice

The performance results concerning Compton scattering in Geant4 9.1 are published in IEEE NSS 2008 proceedings *(F. Longo, L. Pandola and M.G. Pia)*
Geant 4

Born from the requirements of large scale HEP experiments

Widely used also in
- Space science and astronomy
- Medical physics, nuclear medicine
- Radiation protection
- Accelerator physics
- Humanitarian projects, security
- etc.

Technology transfer to industry, hospitals…

Most cited
“Nuclear Science and Technology” publication!
(>140000 papers)

2nd most cited CERN/INFN paper
“Modern classic”

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

Geant4 R&D phase: RD44
- 1994-1998 (Geant4 0.0: 15 December 1998)
- Designed and built Geant4
- New software technology
- GEANT 3 experience + new ideas

Foundation of the current Geant4: dates back to the mid ’90s
- Requirements for core capabilities
- Software technology

Evolution: 1998-2009
- Consolidation, validation, extension and refinement of existing capabilities
- Support to the experimental community
- Proliferation of physics models
- Same core capabilities and technology as in the mid ’90s

1994
mid of LEP era
GEANT 3
successfully used in
many experiments

Collected from the experimental community
Object Oriented methods introduced in HEP

The world changes…
Two worlds...

Condensed-random-walk OR “discrete” régime
- Characterizing choice in a Monte Carlo system
- Limited exception: Penelope (switch to elastic scattering near boundaries)

What does it mean in practice?

How does one estimate radiation effects on components exposed to LHC + detector environment?

And what about nanotechnology-based detectors for HEP?
And tracking in a gaseous detector?
And plasma facing material in a fusion reactor?

How does one link dosimetry to radiation biology?

Subtle consequences
- e.g. X-ray fluorescence emission (PIXE) by impact ionisation has a dependence on secondary production cut introduced to handle infrared divergence!
- can affect macroscopic applications: material analysis, precise dosimetry etc.
Topics of research

R&D study on complementary, co-working transport methods

**Condensed-random-walk** scheme
**Discrete** scheme

**Monte Carlo** method
**Deterministic** methods

- Nanotechnology detectors
- Radiation effects on components
  - Radiobiology
  - Plasma physics
- Material analysis
  - etc.

- Nuclear power plants
  - Radiotherapy
- Homeland security
  - etc.

Side topics (instrumental to the main objectives)

- **Physics configurability**
- **Concerns** (scattered and tangled)
- **Built-in physics V&V-ability**

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R&D on co-working transport schemes in Geant4

Project launched at INFN (2009), international-multidisciplinary team
- **R&D** = research study, exploration of novel ideas
- Distinct from Geant4 production service: no perturbation to running experiments!
- R&D deliverable(s) = prototypes [to be evaluated for transition into Geant4 releases]

Scientific motivation
- From concrete experimental use cases

Objective
- Seamless transition of simulation régime in Geant4
- Capability of simulating complex multi-scale systems

Conceptual and software design challenges
- Physics process adaptation to environment
- Embedding “mutability” in Monte Carlo physics entities

Difficult
- …not yet present in any simulation system
UP: iterative and incremental software process

1st cycle: propedeutic exploration

- Problem domain analysis
  - Identify entities subject to mutability

- Added complexity
  - Deterioration of performance?

- Side requirements
  - Agility of configuration
    - Transparency
    - Easy verification & validation

- Technology
  - Support to requirements

Pilot project: mutability in photon physics domain

R&D on generic programming techniques in EM physics
**Design Style**  
Adopt best practices, build on existing body of knowledge

5. Give one entity one cohesive responsibility.
6. Correctness, simplicity, and clarity come first.
7. Know when and how to code for scalability.
8. Don’t optimize prematurely.
9. Don’t pessimize prematurely.
10. Minimize global and shared data.
11. Hide information.

**Class Design and Inheritance**

32. Be clear what kind of class you’re writing.
33. Prefer minimal classes to monolithic classes.
34. Prefer composition to inheritance.
35. Avoid inheriting from classes that were not designed to be base classes.
36. Prefer providing abstract interfaces.
37. Public inheritance is substitutability. Inherit, not to reuse, but to be reused.
38. Practice safe overriding.
39. Consider making virtual functions nonpublic, and public functions nonvirtual.
40. Avoid providing implicit conversions.
41. Make data members private, except in behaviorless aggregates (C-style structs).
42. Don’t give away your internals.
**Minimlism...**

**Item 18: Strive for class interfaces that are complete and minimal.**

The client interface for a class is the interface that is accessible to the programmers who use the class. Typically, only functions exist in this interface, because having data members in the client interface has a number of drawbacks (see Item 20).

**Item 33: Use inlining judiciously.**

Inline functions — what a wonderful idea! They look like functions, they act like functions, they're ever so much better than macros (see Item 1), and you can call them without having to incur the overhead of a function call. What more could you possibly ask for?
No charged photons

Item 35: Make sure public inheritance models “isa.”

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No nostalgia!

Encapsulation = robustness, transparency

**Item 30:** Avoid member functions that return non-const pointers or references to members less accessible than themselves.

```
G4VEMProcess
  theCutsGamma : const std::vector<G4double>*
  theCutsElectron : const std::vector<G4double>*
  theCutsPositron : const std::vector<G4double>*
  currentCouple : const G4MaterialCutsCouple*
  currentMaterialIndex : size_t
  emModels : std::vector<G4EmModel>*
  theCuts : const std::vector<G4double>*
  deRegions : std::vector<const G4Region>*
  secParticles : std::vector<G4DynamicParticle>*
  PostStepDoIt( : const G4Track&, : const G4Step&) : G4VParticleChange*

G4VEMModel
```

FORTRAN common block...

```
PostStepDoIt
  -currentModel
  currentModel->SampleSecondaries(&secParticles,
      currentCouple,
      track.GetDynamicParticle(),
      (*theCuts)[currentMaterialIndex]);
```

Encapsulation = robustness, transparency

```
G4KleinNishinaCompton
  (from standard)

```
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Design, design, design...

Item 39: Avoid casts down the inheritance hierarchy.

In these tumultuous economic times, it's a good idea to keep an eye on our financial institutions, so consider a Protocol class (see Item 34) for bank accounts:

src/G4BetheBlochModel.cc: fParticleChange = reinterpret_cast<G4ParticleChangeForLoss*>(pParticleChange);
src/G4BetheHeitlerModel.cc: fParticleChange = reinterpret_cast<G4ParticleChangeForGamma*>(pParticleChange);
src/G4BraggIonModel.cc: reinterpret_cast<G4ParticleChangeForLoss*>(pParticleChange);
src/G4BraggModel.cc: reinterpret_cast<G4ParticleChangeForLoss*>(pParticleChange);
src/G4eBremsstrahlungModel.cc: fParticleChange = reinterpret_cast<G4ParticleChangeForLoss*>(pParticleChange);
src/G4eBremsstrahlungRelModel.cc: fParticleChange = reinterpret_cast<G4ParticleChangeForLoss*>(pParticleChange);
src/G4eCoulombScatteringModel.cc: reinterpret_cast<G4ParticleChangeForGamma*>(pParticleChange);
src/G4KleinNishinaCompton.cc: fParticleChange = reinterpret_cast<G4ParticleChangeForGamma*>(pParticleChange);
src/G4MollerBhabhaModel.cc: fParticleChange = reinterpret_cast<G4ParticleChangeForLoss*>(pParticleChange);
src/G4MscModel71.cc: fParticleChange = reinterpret_cast<G4ParticleChangeForMSC*>(pParticleChange);
src/G4MultipleScattering71.cc: model = dynamic_cast<G4MscModel71*>(SelectModel(e));
src/G4PEEffectModel.cc: fParticleChange = reinterpret_cast<G4ParticleChangeForGamma*>(pParticleChange);
src/G4UrbanMscModel2.cc: fParticleChange = reinterpret_cast<G4ParticleChangeForMSC*>(pParticleChange);
src/G4UrbanMscModel90.cc: fParticleChange = reinterpret_cast<G4ParticleChangeForMSC*>(pParticleChange);
src/G4UrbanMscModel.cc: fParticleChange = reinterpret_cast<G4ParticleChangeForMSC*>(pParticleChange);
Policy-based design

A policy defines a class or class template interface

Policy host classes are parameterised classes

Advantages

- Policies are not required to inherit from a base class
- The code is bound at compile time
  - No need of virtual methods, resulting in faster execution

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

Syntax-oriented rather than signature-oriented

Highly customizable design

C++ is capable of a Turing machine at two levels

Exploit both
Mix and match

First introduced in Geant4
S. Chauvie et al.,
Geant4 physics processes for microdosimetry simulation: design foundation and implementation of the first set of models

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minimalism

One entry found.

Main Entry: minimalism
Pronunciation: /ˈmi-nə-məl-əm/
Function: noun
Date: 1929

1: a style or technique (as in music, literature, or design) that is characterized by extreme sparseness and simplicity.
Correctness

- Better control on software correctness
- Easy to unit test physics ingredients

Old Penelope Compton scattering test
Unphysical values

Disappear in the new design
(same test code)

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**Compton cross section % difference**

### Library-Penelope

Si, Z=14

![Graph showing the distribution of Compton cross section differences between Library and Penelope for Si with Z=14.](image)

- **Different scale!**

### Library-Standard

Si, Z=14

![Graph showing the distribution of Compton cross section differences between Library and Standard for Si with Z=14.](image)

- **Different scale!**

### Penelope-Standard

Si, Z=14

![Graph showing the distribution of Compton cross section differences between Penelope and Standard for Si with Z=14.](image)

- **Different scale!**

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**χ² test NIST Phys. Ref. Data**

<table>
<thead>
<tr>
<th></th>
<th>p-value</th>
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</thead>
<tbody>
<tr>
<td>Library</td>
<td>0.982</td>
</tr>
<tr>
<td>Penelope</td>
<td>&lt;0.001</td>
</tr>
<tr>
<td>Standard</td>
<td>0.189</td>
</tr>
</tbody>
</table>

- **0.993 excluding 1 keV**
K. Amako et al.,
Comparison of Geant4 electromagnetic physics models against the NIST reference data

Old G4-NIST comparison test

- 4134 LoC*
- $O(months)$ CPU+human time

Test with new design

- <50 LoC*, $O(minutes)$
Physics on a diet

The design exposes the physics at very fine granularity
- Cross sections
- Final state detail
- Unprecedented opportunity for thorough validation (where data exist)

Similarities and differences among various Geant4 models
- Accuracy
- Computational performance

Some models provide identical functionality
- Often the result of evolution: initially they were different!

Toolkit nature of Geant4: provide alternative models
- Replicas of the same physics functionality?
- Pruning keeps trees healthier!

Cost of maintenance of a still growing, complex software system
- Long time scale of LHC operation (various developers will be retired)

Strive for simplicity, transparency, sound design, quality of software

Hidden treasures
e.g. 3 variants of atomic binding energies
(1 experimentally validated)

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Performance improvement
(where no improvement is expected)

Example: Penelope Compton

NO ATTEMPT [yet] TO IMPROVE THE IMPLEMENTATION

40 keV, \(10^6\) events, Intel Core2 Duo Processor E6420, 2.13 GZ, 4 GB RAM

<table>
<thead>
<tr>
<th>Material</th>
<th>Policy-based design</th>
<th>Geant4 9.1</th>
<th>Gain</th>
</tr>
</thead>
<tbody>
<tr>
<td>C</td>
<td>4.15</td>
<td>6.08</td>
<td>32%</td>
</tr>
<tr>
<td>Si</td>
<td>6.23</td>
<td>8.37</td>
<td>26%</td>
</tr>
<tr>
<td>Cu</td>
<td>7.64</td>
<td>10.78</td>
<td>29%</td>
</tr>
<tr>
<td>W</td>
<td>14.06</td>
<td>19.18</td>
<td>27%</td>
</tr>
</tbody>
</table>

Move lowenergy-Penelope to Standard package design: ~10% gain, including implementation improvements

Source: L. Pandola, [http://workgroup.lngs.infn.it/geant4lns/group-meetings-directory/l.pandola](http://workgroup.lngs.infn.it/geant4lns/group-meetings-directory/l.pandola)

Low Energy – Library: 28% gain with policy-based design
Doppler broadening in Compton scattering

Si, 40 keV

Cs, 400 keV

Validation on experimental data by Namito et al.

Library Penelope Standard final state Generators

Yes, physics does make sense. And is transparently exposed.

There is only the fight to recover what has been lost
And found and lost again and again: and now, under conditions
That seem unpropitious.

T.S. Eliot, Four Quartets (East Coker)
First considerations

The technology looks promising for application to a large, complex, computationally intensive physics simulation domain.

Enormous gain in
- Transparency
- Agility
- Easy verification and validation
- Maintenance effort

Significant performance improvement
- At a very early stage of the project, still room for further improvement

But there is still a long way to go…

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Outlook

Now the fun begins…

Charged particles

Path towards introducing mutation “in the guts”
Side opportunities for physics improvements, validation, consistency etc. thanks to the transparency of the design

Validation of the design “on the field”
— Collaboration with experimental groups

In my end is my beginning

T.S. Eliot, Four Quartets (East Coker)
Conclusion

Curiosity

Physics

insight

Freedom

Much madness is divinest Sense -
To a discerning Eye -
Much sense - the starkest Madness -
'Tis the Majority
In this, as All, prevails -
Assent - and you are sane -
Demur - you're straightway dangerous -
And handled with a Chain.

Emily Dickinson

Software engineering

discipline

Methodological

rigorousness
Nuclear Science Symposium

25 – 31 October, 2009

The Nuclear Science Symposium (NSS) offers an outstanding opportunity for scientists and engineers interested or actively working in the fields of nuclear science, radiation instrumentation, software and their applications, to meet and discuss with colleagues from around the world. The program emphasizes the latest developments in technology and instrumentation and their implementation in experiments for space, accelerators, other radiation environments, and homeland security. Topical Workshops cover areas of specific interest. Within the framework of an educational scientific program, Short Courses are organized focusing on topics of interest for the scientific community. Authors are invited to submit papers describing original unpublished works in the topics areas listed below:

- Accelerators and Beam Line Instrumentation
- Analog and Digital Circuits
- Astrophysics and Space Instrumentation
- Computing and Software for Experiments
- Data Acquisition and Analysis Systems
- Gamma-ray Imaging
- Gaseous Detectors
- High Energy Physics Instrumentation
- Instrumentation for Homeland Security
- Instrumentation for Medical and Biological Research
- Neutron Imaging and Radiography
- New Detector Concepts and Instrumentation
- Nuclear Measurements and Monitoring Techniques
- Nuclear Physics Instrumentation
- Nuclear Power
- Photodetectors and Scintillation Detectors
- Radiation Damage Effects