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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)
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  - **Alessandro Montanari** (INFN Bologna)
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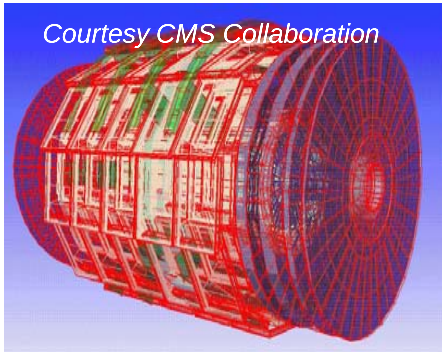
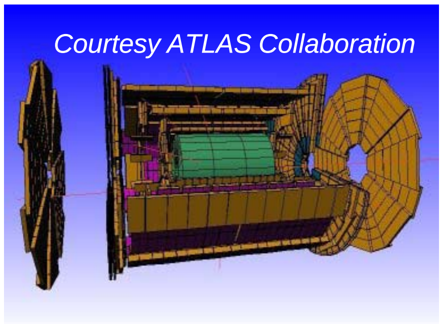
  for helpful discussions and advice

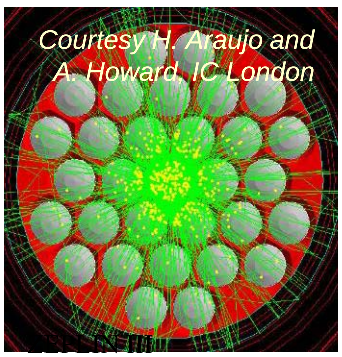
- The performance results concerning Compton scattering in Geant4 9.1 are published in IEEE NSS 2008 proceedings *(F. Longo, L. Pandola and M.G. Pia)*



Courtesy CMS Collaboration



Courtesy ATLAS Collaboration



Courtesy H. Araujo and A. Howard, IC London

Geant 4

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

Born from the requirements of large scale HEP experiments

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

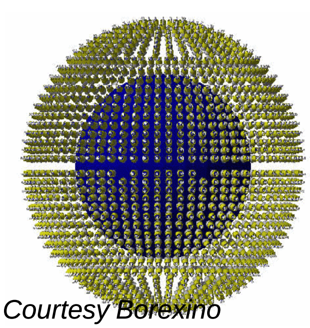
2nd most cited CERN/INFN paper

"Modern classic"

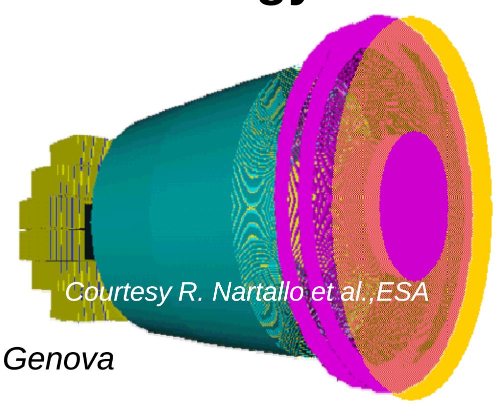
Widely used also in

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

Technology transfer to industry, hospitals…

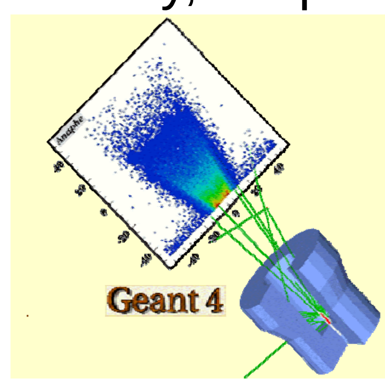


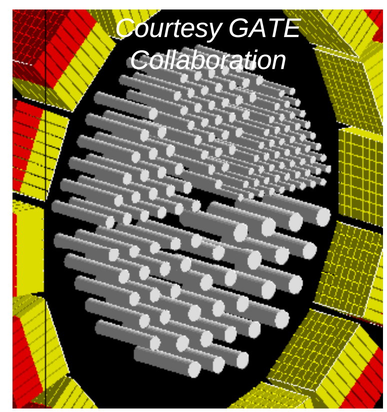
Courtesy Borexino



Courtesy R. Nartallo et al.,ESA

INFN Genova





Courtesy GATE Collaboration

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

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

- **Foundation of the current Geant4: dates back to the mid '90s**
  - Requirements for core capabilities ← Collected from the experimental community
  - Software technology ← Object Oriented methods introduced in HEP

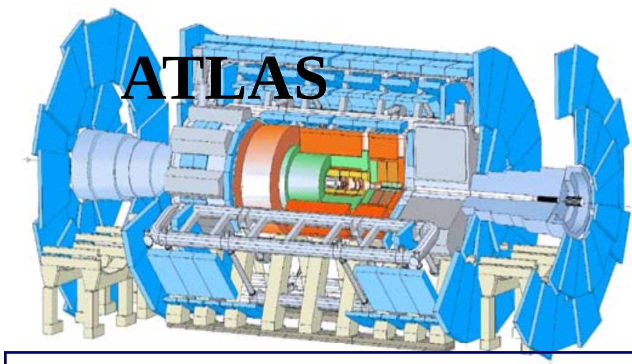
- Evolution: **1998-2009**
  - Consolidation, validation, extension and refinement of existing capabilities
  - Support to the experimental community
  - Proliferation of physics models
  - Same **core capabilities** and **technology** as in the **mid '90s**

The world changes…

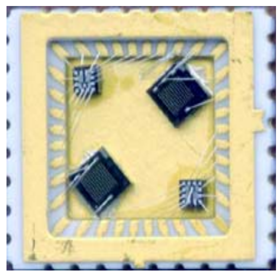
Two worlds...

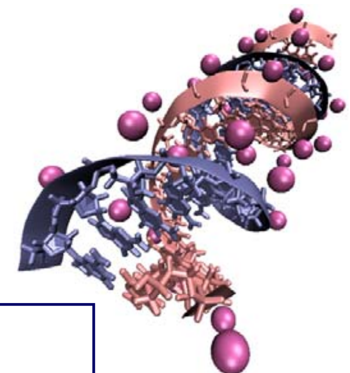
- **Condensed-random-walk OR "discrete" régime**
  - Characterizing choice in a Monte Carlo system
  - Limited exception: Penelope (switch to elastic scattering near boundaries)

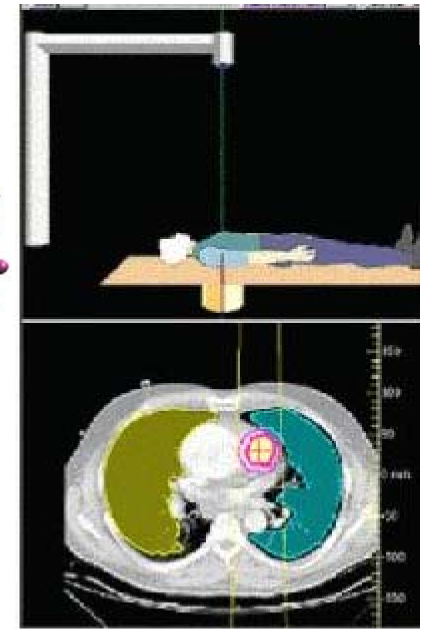
What does it mean in practice?



RADMON







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

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

Monte Carlo method
Deterministic methods

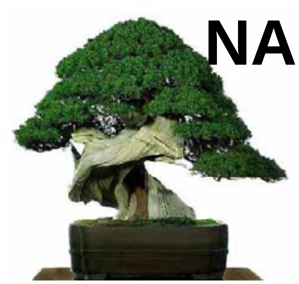
Nuclear power plants
Radiotherapy
Homeland security
etc.

Side topics (instrumental to the main objectives)

Physics configurability

Concerns
(scattered and tangled)

Built-in physics V&V-ability



NANO5

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

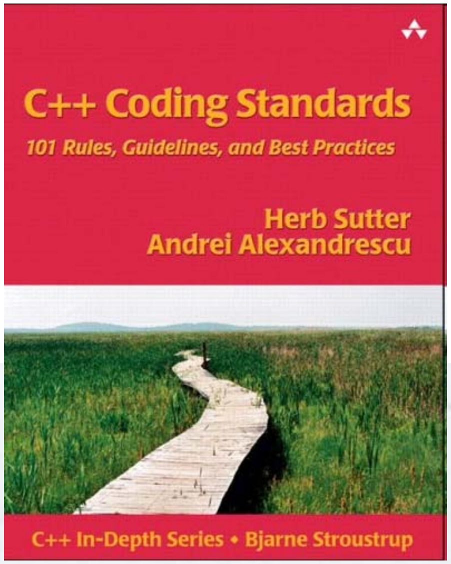
Pilot project: mutability in photon physics domain

R&D on generic programming techniques in EM physics

Adopt best practices, build on existing body of knowledge

Design Style

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.



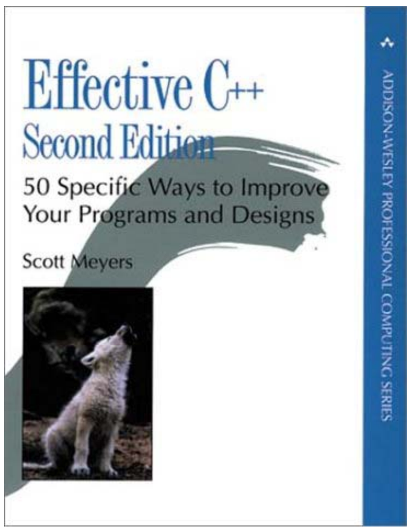
Class Design and Inheritance

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.

Minimalism…

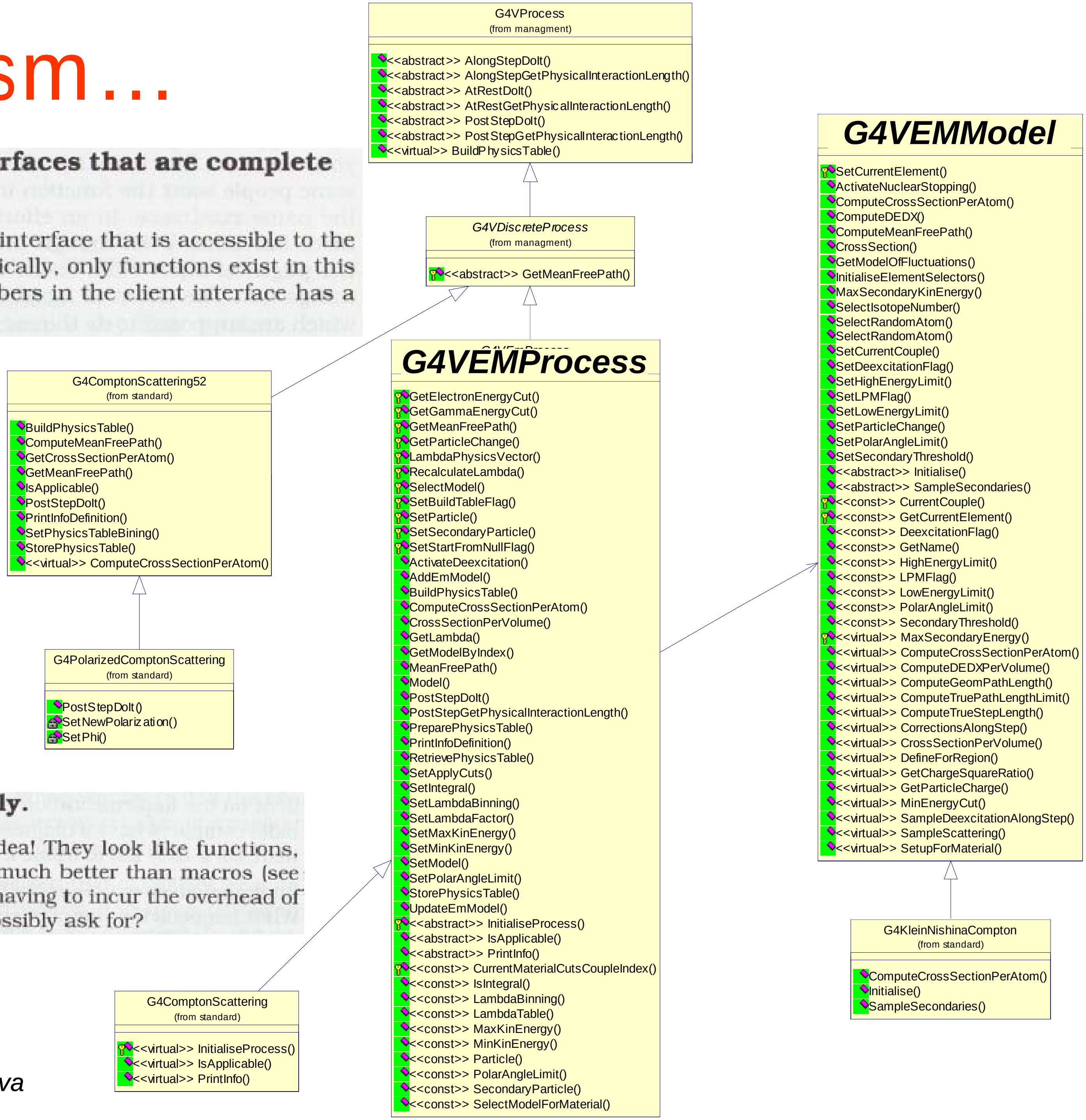
Item 18: Strive for class interfaces that are complete and minimal.

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).



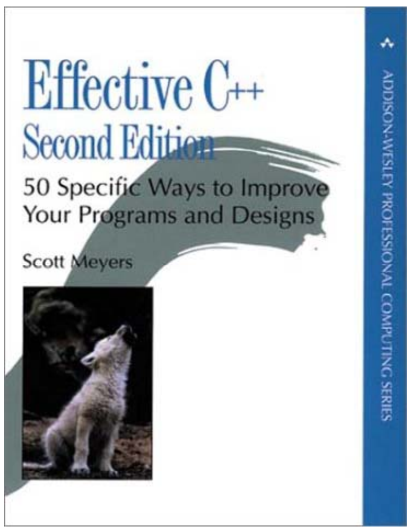
Item 33: Use inlining judiciously.

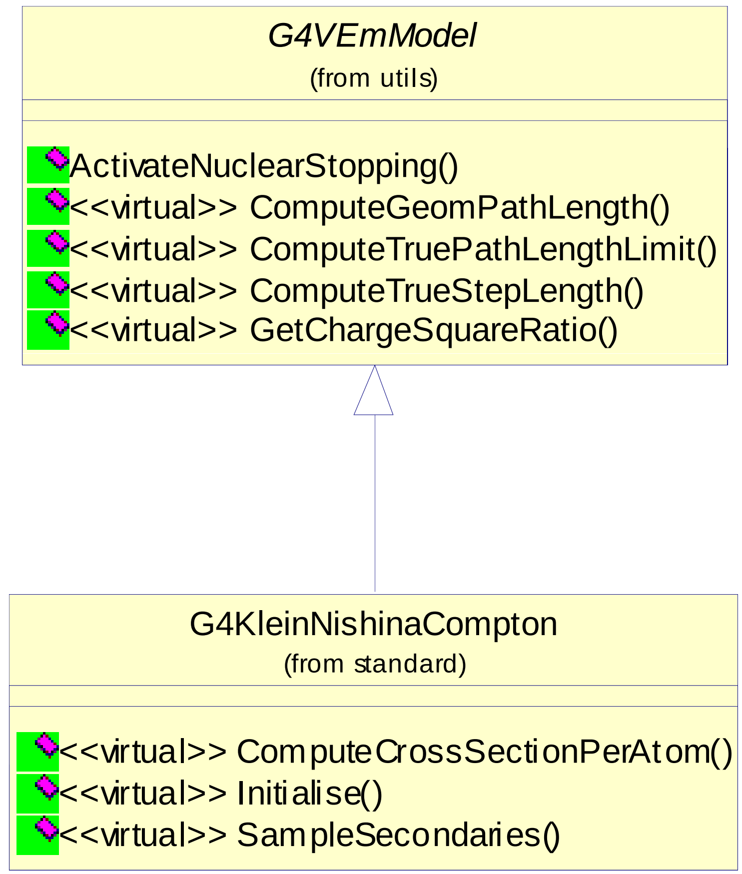
Inline functions — what a *wonderful* idea! They look like functions, they act like functions, they're ever so much better than macros (see Item 1), and you can call them without having to incur the overhead of a function call. What more could you possibly ask for?



No charged photons

Item 35: Make sure public inheritance models "isa."

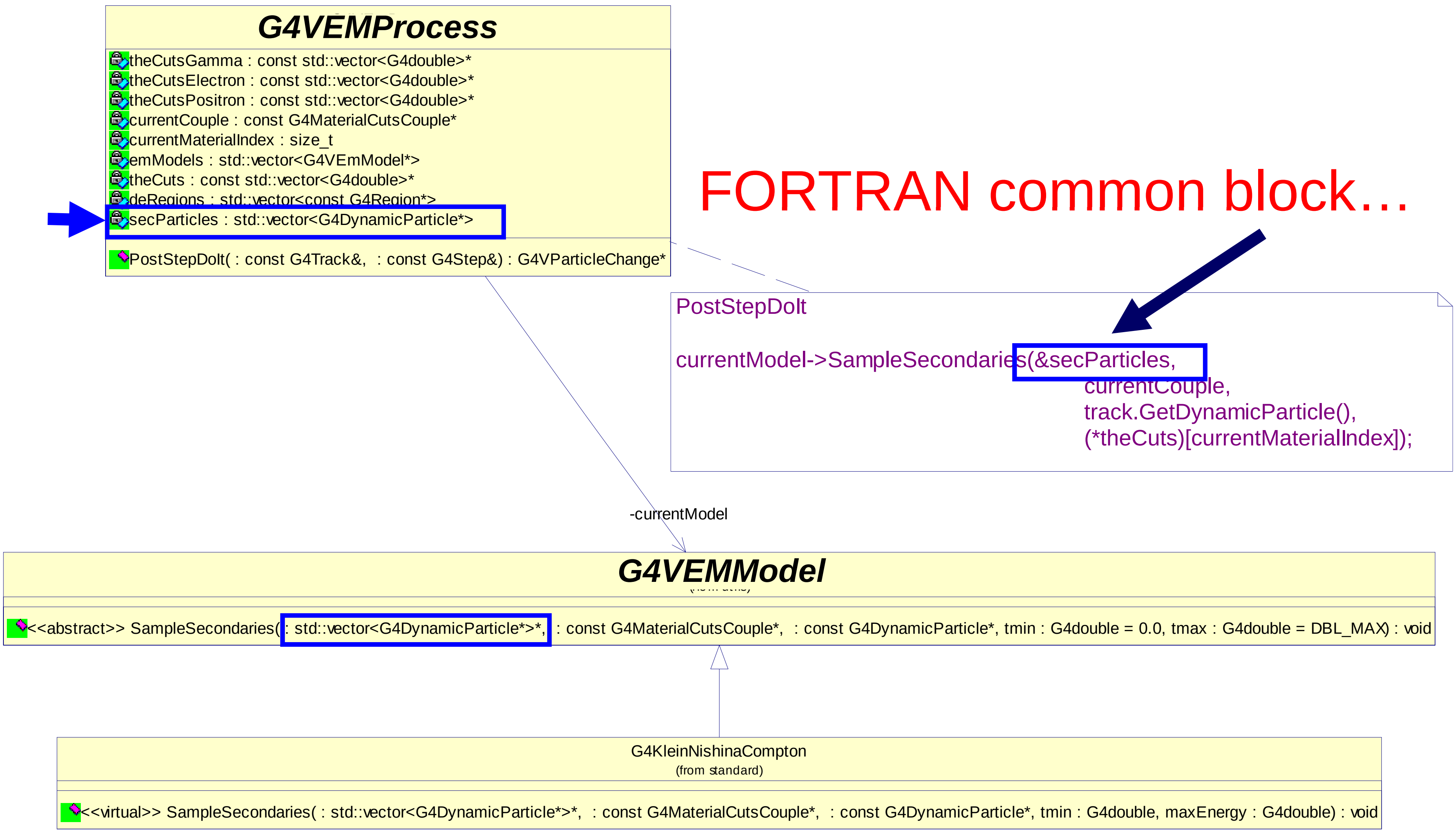


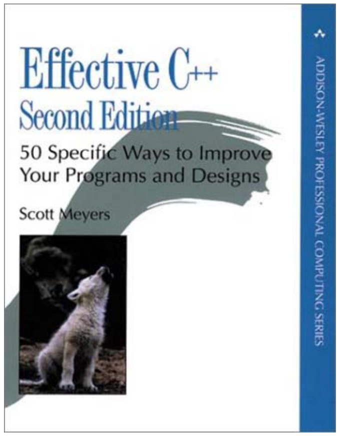


No nostalgia!

Encapsulation = robustness, transparency

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





Design, design, design…

Item 39: Avoid casts down the inheritance hierarchy.

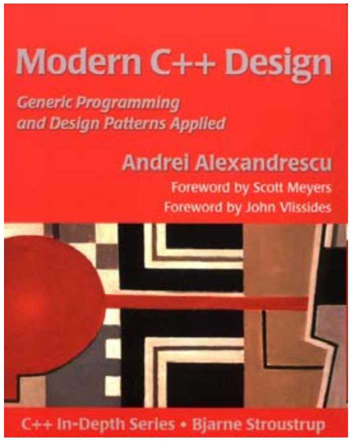
In these tumultuous economic times, it's a good idea to keep an eye on our financial institutions, so consider a Protocol class (see Item 34) for bank accounts:

```
src/G4BetheBlochModel.cc:      fParticleChange = reinterpret_cast<G4ParticleChangeForLoss*>
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*>
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

R&D!

- 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

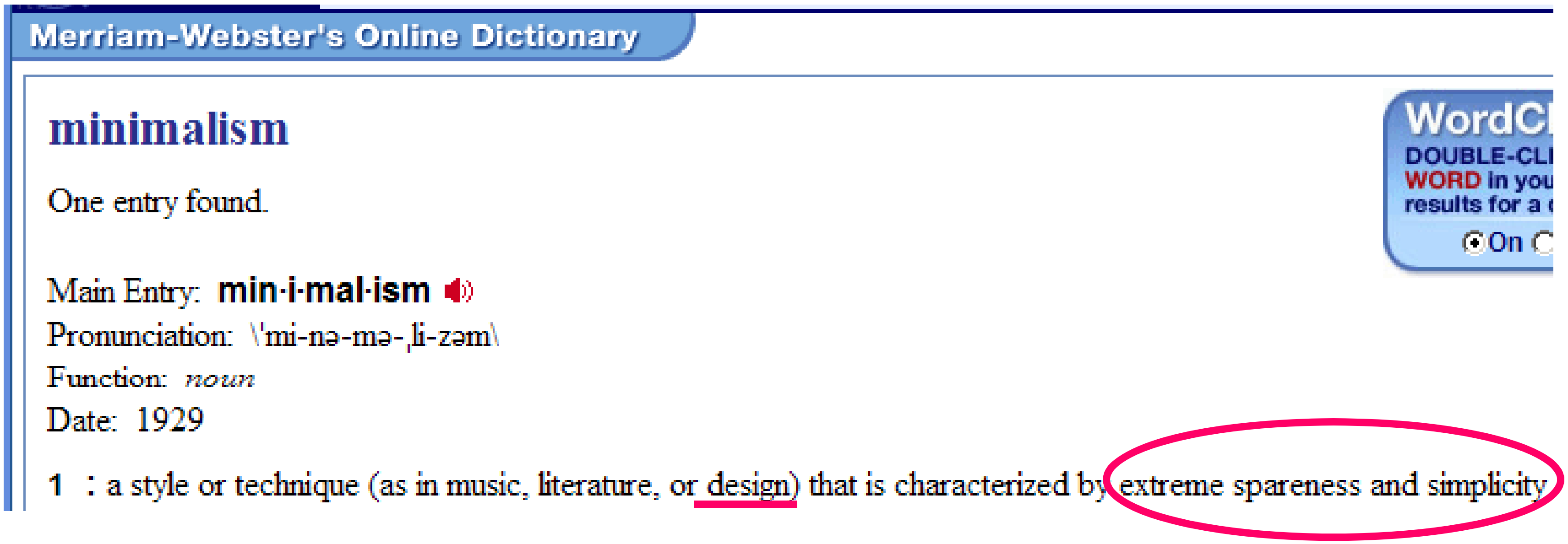
⇩

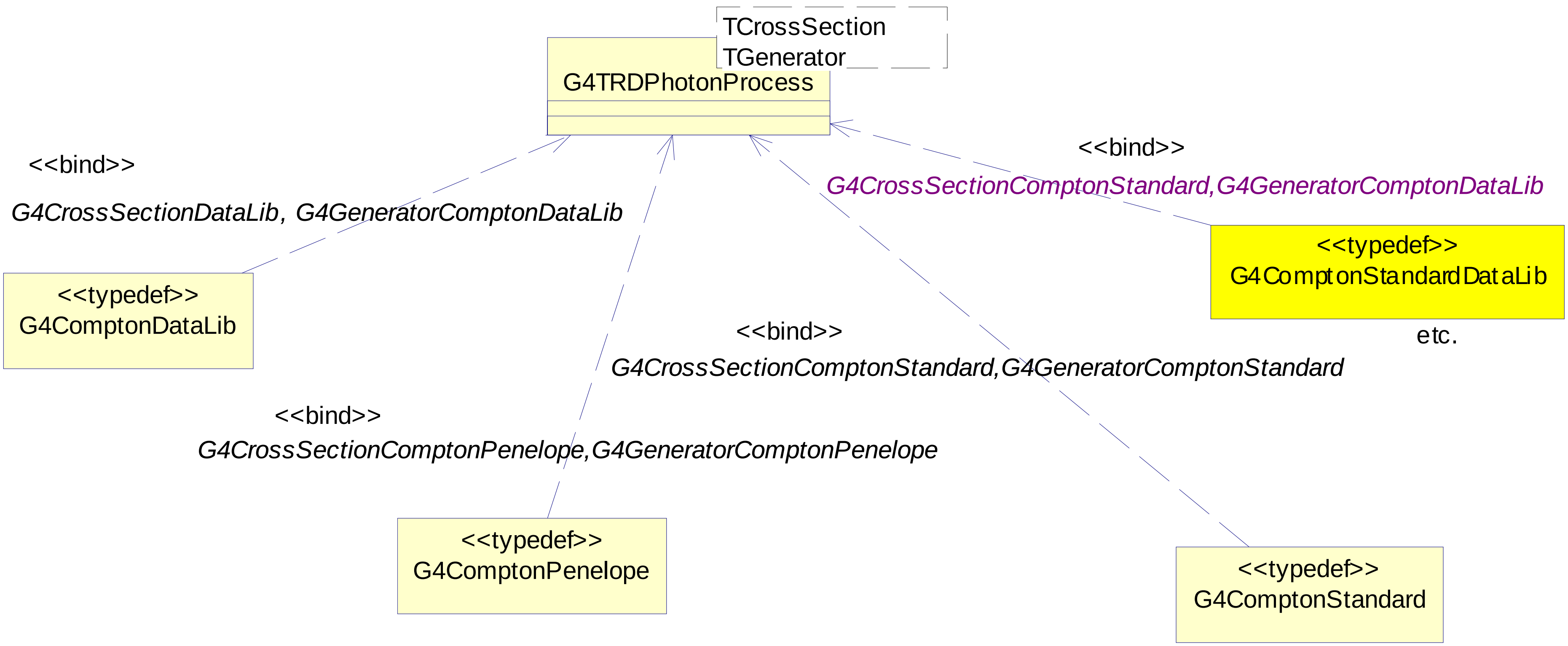
Highly **customizable** design

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

First introduced in Geant4
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

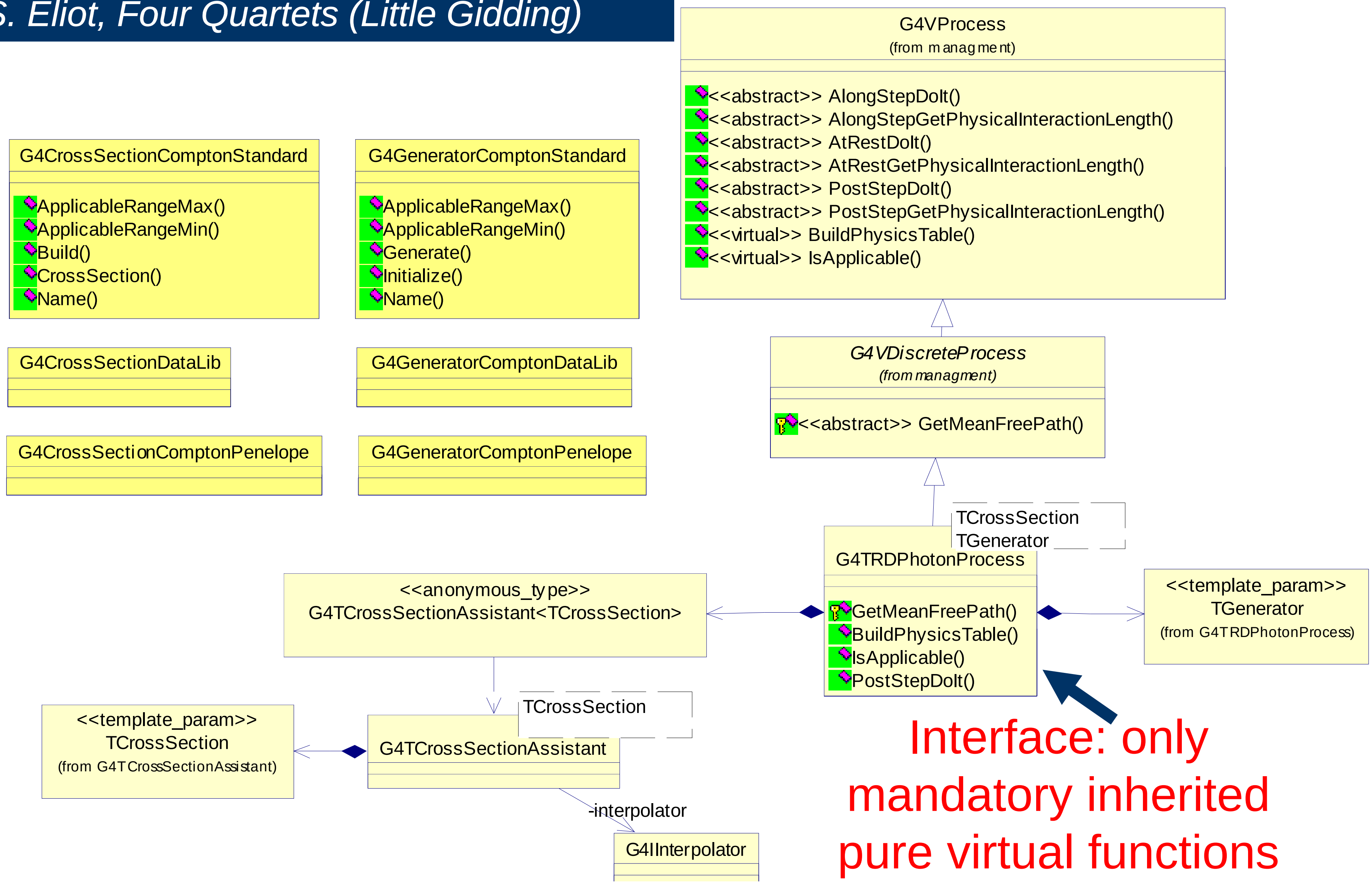
Exploit both
Mix and match


Merriam-Webster's Online Dictionary
minimalism
One entry found.
Main Entry: min·i·mal·ism
Pronunciation: \ˈmi-nə-mə-ˌli-zəm\
Function: noun
Date: 1929
1 : a style or technique (as in music, literature, or design) that is characterized by extreme spareness and simplicity
WordCl
DOUBLE-CLI
WORD in you
results for a
On


TCrossSection
TGenerator
G4TRDPhotonProcess
<<bind>>
G4CrossSectionDataLib, G4GeneratorComptonDataLib
<<bind>>
G4CrossSectionComptonStandard,G4GeneratorComptonDataLib
<<typedef>>
G4ComptonStandardDataLib
<<typedef>>
G4ComptonDataLib
<<bind>>
G4CrossSectionComptonStandard,G4GeneratorComptonStandard
etc.
<<bind>>
G4CrossSectionComptonPenelope,G4GeneratorComptonPenelope
<<typedef>>
G4ComptonPenelope
<<typedef>>
G4ComptonStandard

A condition of complete simplicity (Costing not less than everything)

T.S. Eliot, Four Quartets (Little Gidding)



Interface: only mandatory inherited pure virtual functions

typedef G4PhotonProcess<G4CrossSectionComptonStandard,G4GeneratorComptonStandard> G4ComptonStandard>

Correctness

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

Old Penelope Compton scattering test

Unphysical values

Disappear in the new design

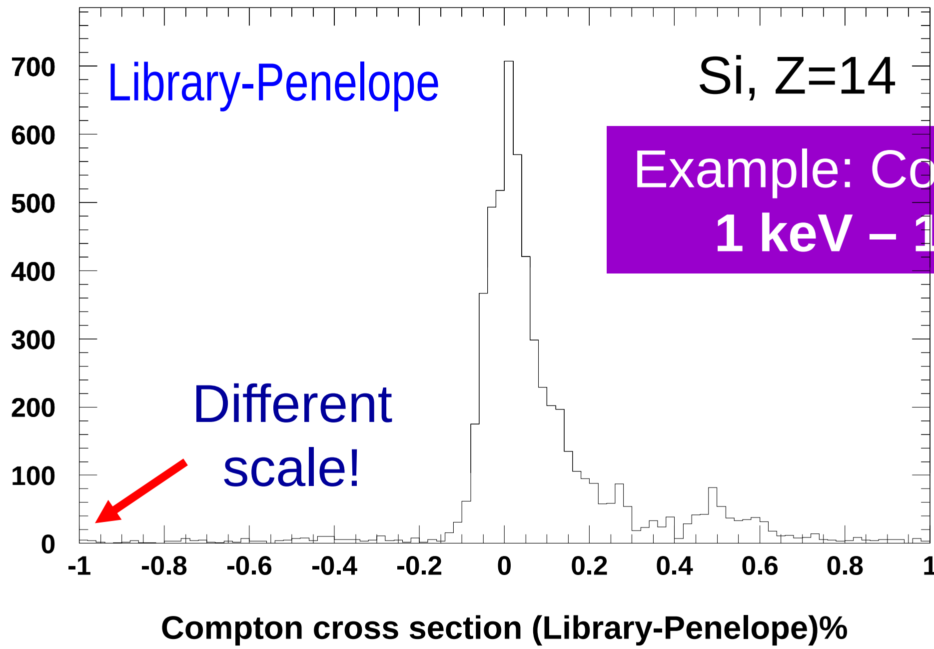
(same test code)

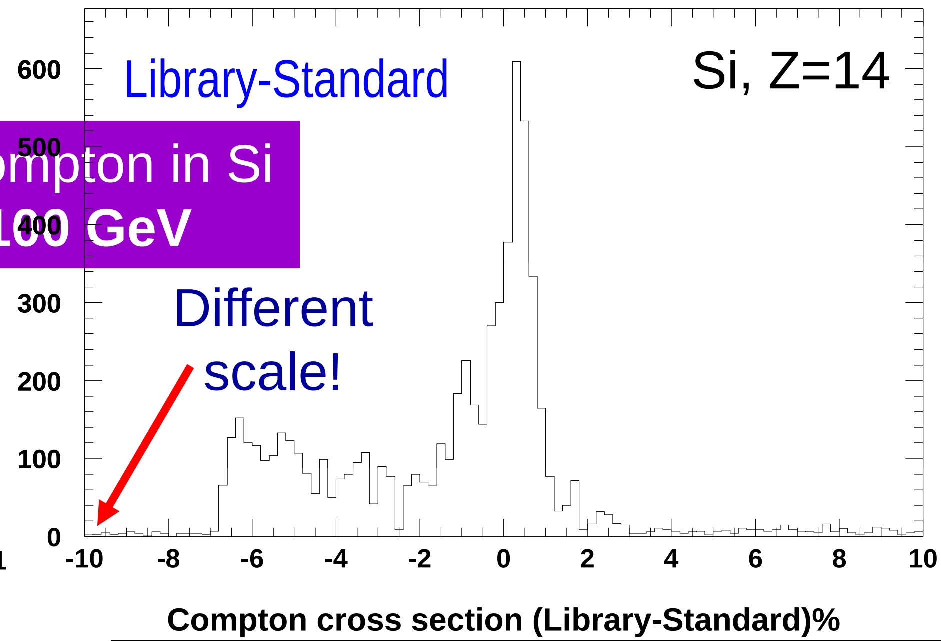
```
G4VParticleChange::CheckSecondary  :   the kinetic energy is negative  !!
 Difference:  1.34307e-06[MeV]
G4VParticleChange::CheckSecondary  :   the kinetic energy is negative  !!
 Difference:  2.05246e-06[MeV]
G4VParticleChange::CheckSecondary  :   the kinetic energy is negative  !!
 Difference:  3.96231e-06[MeV]
G4VParticleChange::CheckSecondary  :   the kinetic energy is negative  !!
 Difference:  1.93648e-07[MeV]
G4VParticleChange::CheckSecondary  :   the kinetic energy is negative  !!
 Difference:  4.08706e-06[MeV]
G4VParticleChange::CheckSecondary  :   the kinetic energy is negative  !!
 Difference:  3.04296e-06[MeV]
G4VParticleChange::CheckSecondary  :   the kinetic energy is negative  !!
 Difference:  8.2724e-07[MeV]
G4VParticleChange::CheckSecondary  :   the kinetic energy is negative  !!
 Difference:  1.16916e-06[MeV]
G4VParticleChange::CheckSecondary  :   the kinetic energy is negative  !!
 Difference:  1.92611e-06[MeV]
G4VParticleChange::CheckSecondary  :   the kinetic energy is negative  !!
 Difference:  9.10367e-07[MeV]
G4VParticleChange::CheckSecondary  :   the kinetic energy is negative  !!
 Difference:  1.53518e-06[MeV]
G4VParticleChange::CheckSecondary  :   the kinetic energy is negative  !!
 Difference:  1.04098e-06[MeV]
G4VParticleChange::CheckSecondary  :   the kinetic energy is negative  !!
 Difference:  4.03171e-07[MeV]
G4VParticleChange::CheckSecondary  :   the kinetic energy is negative  !!
 Difference:  2.51591e-06[MeV]
G4VParticleChange::CheckSecondary  :   the kinetic energy is negative  !!
 Difference:  3.20594e-07[MeV]
G4VParticleChange::CheckSecondary  :   the kinetic energy is negative  !!
 Difference:  6.80522e-08[MeV]
G4VParticleChange::CheckSecondary  :   the kinetic energy is negative  !!
 Difference:  9.55836e-07[MeV]
G4VParticleChange::CheckSecondary  :   the kinetic energy is negative  !!
 Difference:  4.13628e-06[MeV]
G4VParticleChange::CheckSecondary  :   the kinetic energy is negative  !!
 Difference:  1.03676e-06[MeV]
G4VParticleChange::CheckSecondary  :   the kinetic energy is negative  !!
 Difference:  2.82759e-06[MeV]
G4VParticleChange::CheckSecondary  :   the kinetic energy is negative  !!
 Difference:  4.75401e-06[MeV]
G4VParticleChange::CheckSecondary  :   the kinetic energy is negative  !!
 Difference:  5.60175e-07[MeV]
G4VParticleChange::CheckSecondary  :   the kinetic energy is negative  !!
 Difference:  3.69911e-08[MeV]
G4VParticleChange::CheckSecondary  :   the kinetic energy is negative  !!
 Difference:  7.15749e-07[MeV]
G4VParticleChange::CheckSecondary  :   the kinetic energy is negative  !!
```

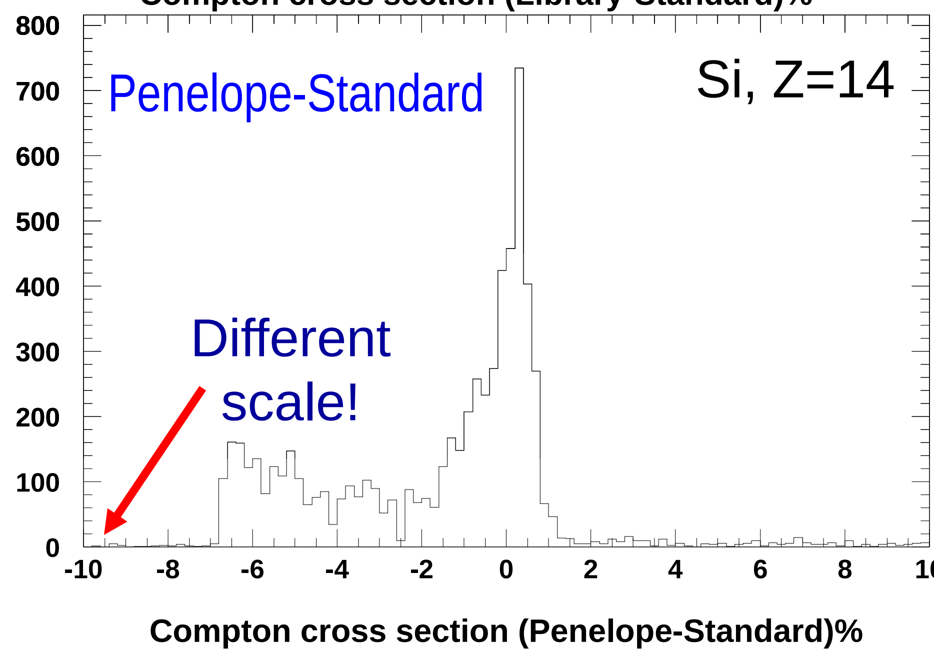
Compton cross section % difference

Agility

Example: Compton in Si
1 keV – 100 GeV







χ^2 test NIST Phys. Ref. Data

	p-value
Library	0.982
Penelope	<0.001 *0.993 excluding 1 keV*
Standard	0.189

Metrics

Photon cross sections test

K. Amako et al.,
Comparison of Geant4 electromagnetic physics models against the NIST reference data
IEEE Trans. Nucl. Sci., vol. 52, no. 4, pp. 910-918, Aug. 2005

Old G4-NIST comparison test

4134 LoC*
O(months) CPU+human time

```
MGpcpia2 > ls include
CVS                            Tst50ElectronEEDLrange.hh      Tst50PhotonStandard.hh                Tst50ProtonStandard.hh
Tst50AlphaICRU49.hh            Tst50ElectronPenelope.hh       Tst50PhysicsList.hh                   Tst50ProtonZiegler2000.hh
Tst50AlphaStandard.hh          Tst50ElectronStandardback.hh   Tst50PhysicsListMessenger.hh          Tst50ProtonZiegler85.hh
Tst50AlphaZiegler.hh           Tst50ElectronStandard.hh       Tst50PositronPenelope.hh              Tst50RunAction.hh
Tst50AnalysisManager.hh        Tst50EventAction.hh            Tst50PositronStandardBack.hh          Tst50RunMessenger.hh
Tst50DetectorConstruction.hh   Tst50Particles.hh              Tst50PositronStandard.hh              Tst50SteppingAction.hh
Tst50DetectorMessenger.hh      Tst50PhotonEPDL.hh             Tst50PrimaryGeneratorAction.hh        Tst50SteppingVerbose.hh
Tst50ElectronEEDLback.hh       Tst50PhotonPenelope.hh         Tst50PrimaryGeneratorMessenger.hh     Tst50TrackerHit.hh
Tst50ElectronEEDL.hh           Tst50PhotonPolarised.hh        Tst50ProtonICRU49.hh                  Tst50TrackerSD.hh
MGpcpia2 > ls src
CVS                            Tst50ElectronEEDLrange.cc      Tst50PhotonStandard.cc                Tst50ProtonStandard.cc
Tst50AlphaICRU49.cc            Tst50ElectronPenelope.cc       Tst50PhysicsList.cc                   Tst50ProtonZiegler2000.cc
Tst50AlphaStandard.cc          Tst50ElectronStandardback.cc   Tst50PhysicsListMessenger.cc          Tst50ProtonZiegler85.cc
Tst50AlphaZiegler.cc           Tst50ElectronStandard.cc       Tst50PositronPenelope.cc              Tst50RunAction.cc
Tst50AnalysisManager.cc        Tst50EventAction.cc            Tst50PositronStandardBack.cc          Tst50RunMessenger.cc
Tst50DetectorConstruction.cc   Tst50Particles.cc              Tst50PositronStandard.cc              Tst50SteppingAction.cc
Tst50DetectorMessenger.cc      Tst50PhotonEPDL.cc             Tst50PrimaryGeneratorAction.cc        Tst50SteppingVerbose.cc
Tst50ElectronEEDLback.cc       Tst50PhotonPenelope.cc         Tst50PrimaryGeneratorMessenger.cc     Tst50TrackerHit.cc
Tst50ElectronEEDL.cc           Tst50PhotonPolarised.cc        Tst50ProtonICRU49.cc                  Tst50TrackerSD.cc
MGpcpia2 > ls
CVS  default.mac  GNUmakefile  History  include  README  src  test50.cc  test50.in  test_input_files
```

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)*

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

- **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

Performance improvement
(where no improvement is expected)

Example: **Penelope Compton**

Preliminary

NO ATTEMPT [yet] TO IMPROVE THE IMPLEMENTATION

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

	Policy-based design	Geant4 9.1	Gain
C	4.15	6.08	32%
Si	6.23	8.37	26%
Cu	7.64	10.78	29%
W	14.06	19.18	27%

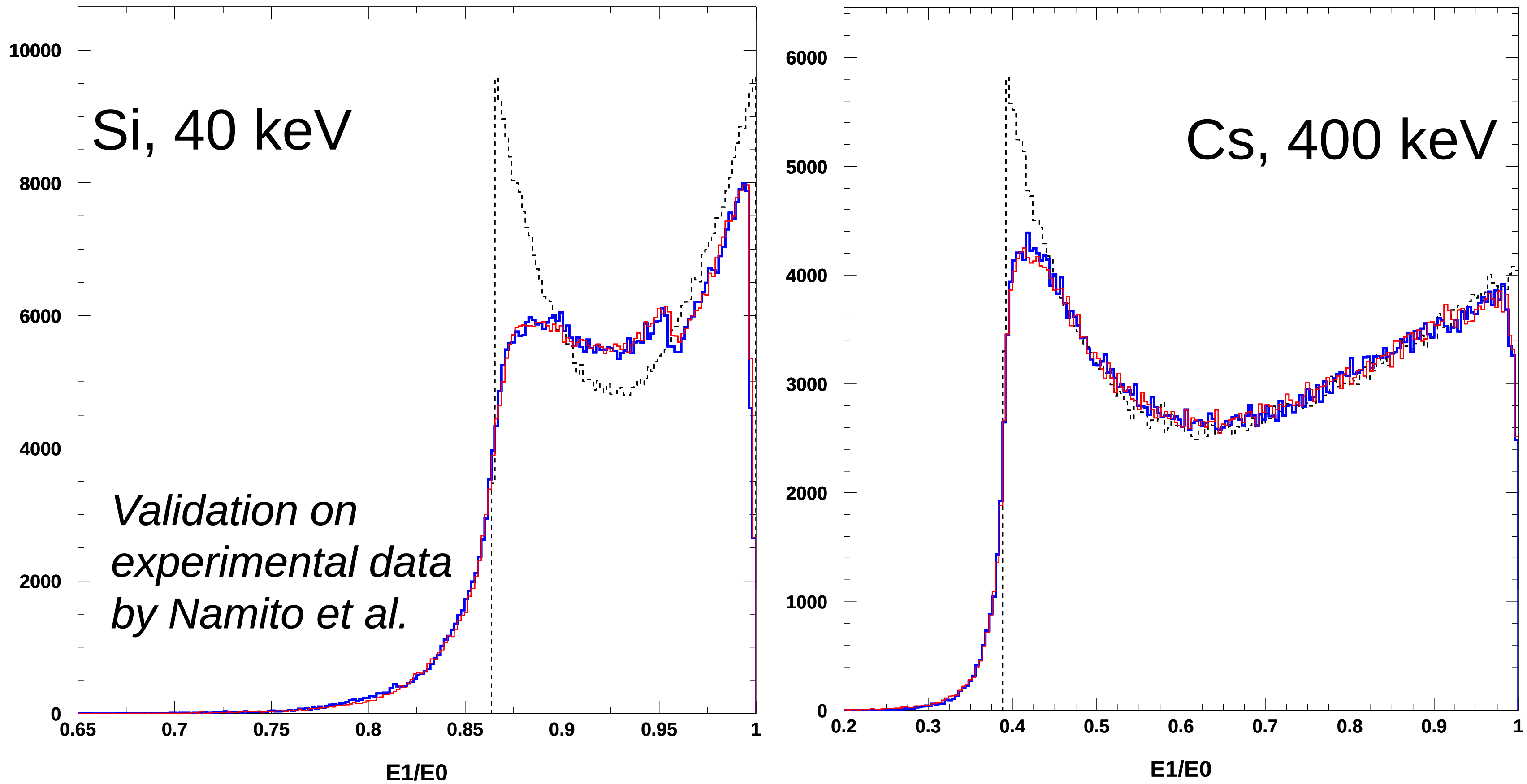
Move lowenergy-Penelope to Standard package design: ~10% gain, including implementation improvements

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

Low Energy – Library: 28% gain with policy-based design

> 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)*

Doppler broadening in Compton scattering



Library Penelope Standard final state Generators

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

The only wisdom we can hope to acquire
Is the wisdom of humility: humility is endless.
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…

And so each venture
Is a new beginning *T.S. Eliot, Four Quartets (East Coker)*

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
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Nuclear Science Symposium

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- Computing and Software for Experiments
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- 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