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Testable physics by design

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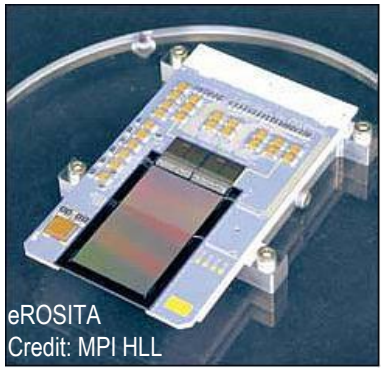
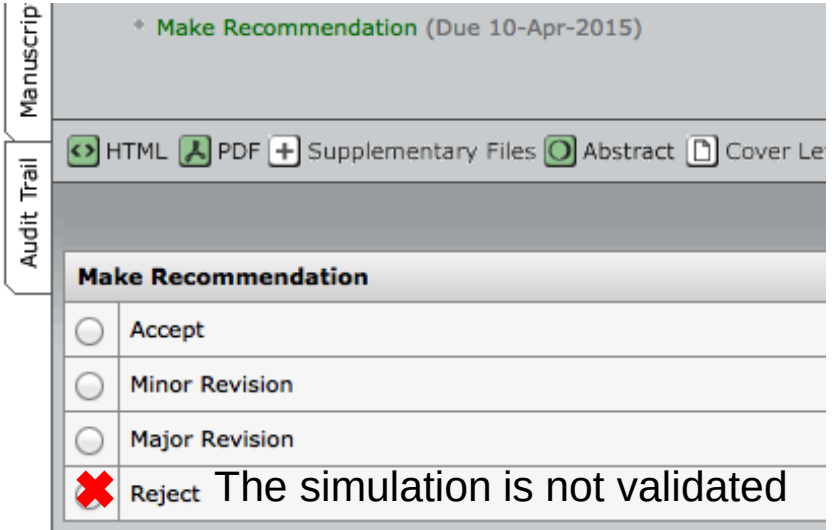
Foreword

Due to limited time allocation, there is room to highlight concepts only
Details will be documented and discussed in a dedicated journal publication

I have a dream…





In the literature…

- Limited documentation of **simulation validation**
  - Mostly in the form of specific use cases compared to measurements in the same experimental scenario
    - Do they apply to similar/different use cases?
    - How to extrapolate the results to different scenarios?

(quantitative)

- Hardly any **validation of the basic physics models** implemented in Monte Carlo codes
  - Why?
- Ongoing projects on **uncertainty quantification**
  - See CHEP 2013, P. Saracco et al.
  - Methods to predict the uncertainty of simulation observables based on knowledge of the uncertainties of simulation "ingredients"

You need an experiment to test a cross section

Testing total cross sections calculated by *G4PEEffectFluoModel*

You can find the photoelectric cross section *G4PEEffectFluoModel* class in $G4INSTALL/source/processes/electromagnetic/standard/include (*G4PEEffectFluoModel.hh* header file) and $G4INSTALL/source/processes/electromagnetic/standard/src/ (*G4PEEffectFluoModel.cc* implementation). *G4PEEffectFluoModel* has a *ComputeCrossSsectionPerAtom* public member function, which returns the total photoelectric cross section for a given element corresponding to a given photon energy:

```
G4double ComputeCrossSectionPerAtom(const G4ParticleDefinition*,
                                    G4double kinEnergy,
                                    G4double Z,
                                    G4double A,
                                    G4double, G4double)
```

Geant4 photoelectric cross section

This is what we need indeed!

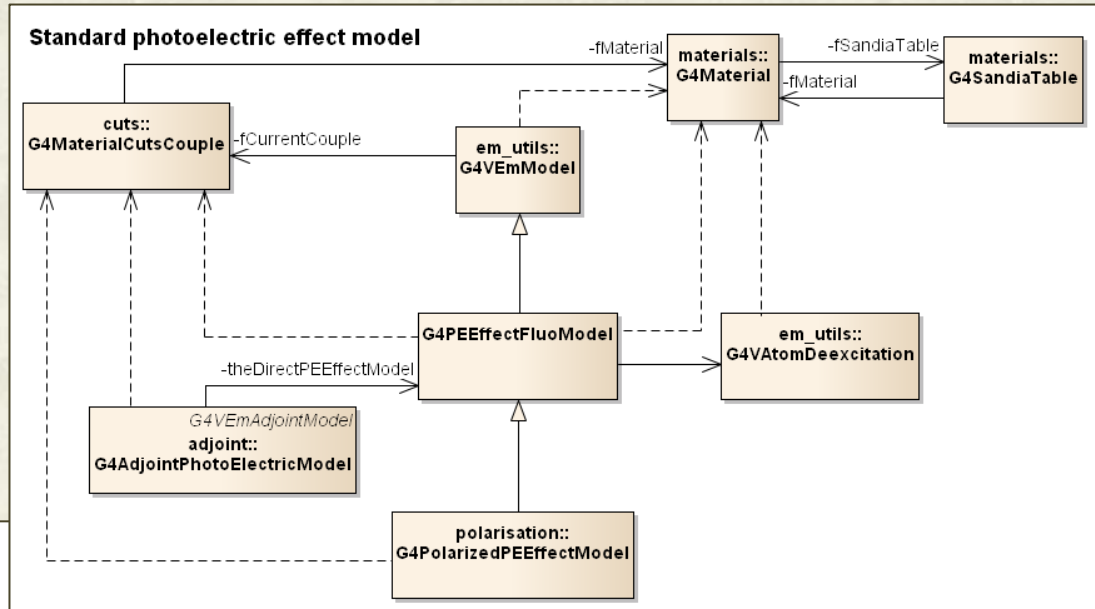
We create a simple unit test *G4PEEffectFluoModelTest.cc*, which instantiates a *G4PEEffectFluoModel* object and invokes *ComputeCrossSectionPerAtom* in pre-defined configurations of photon energy and target element. We place the unit test in $APCDIR/test.

We build the test:

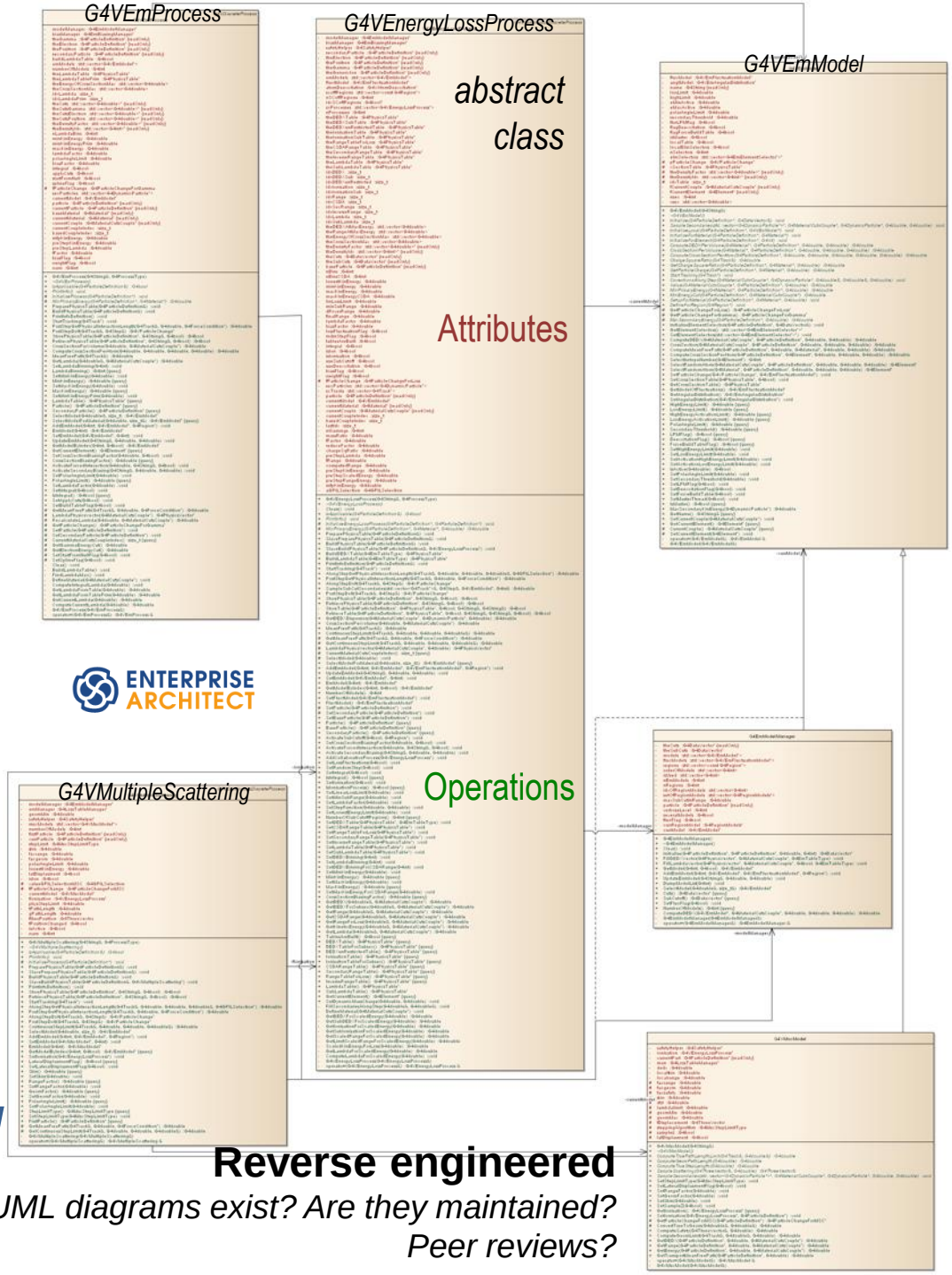
```
cd $APCDIR/test
setenv TESTTARGET G4PEEffectFluoModelTest
gmake
```

Then we **run the test:**

```
$G4WORKDIR/bin/Linux-g++/G4PEEffectFluoModelTest
```



Post-RD44 electromagnetic software design



Hidden dependencies

on other parts of the software

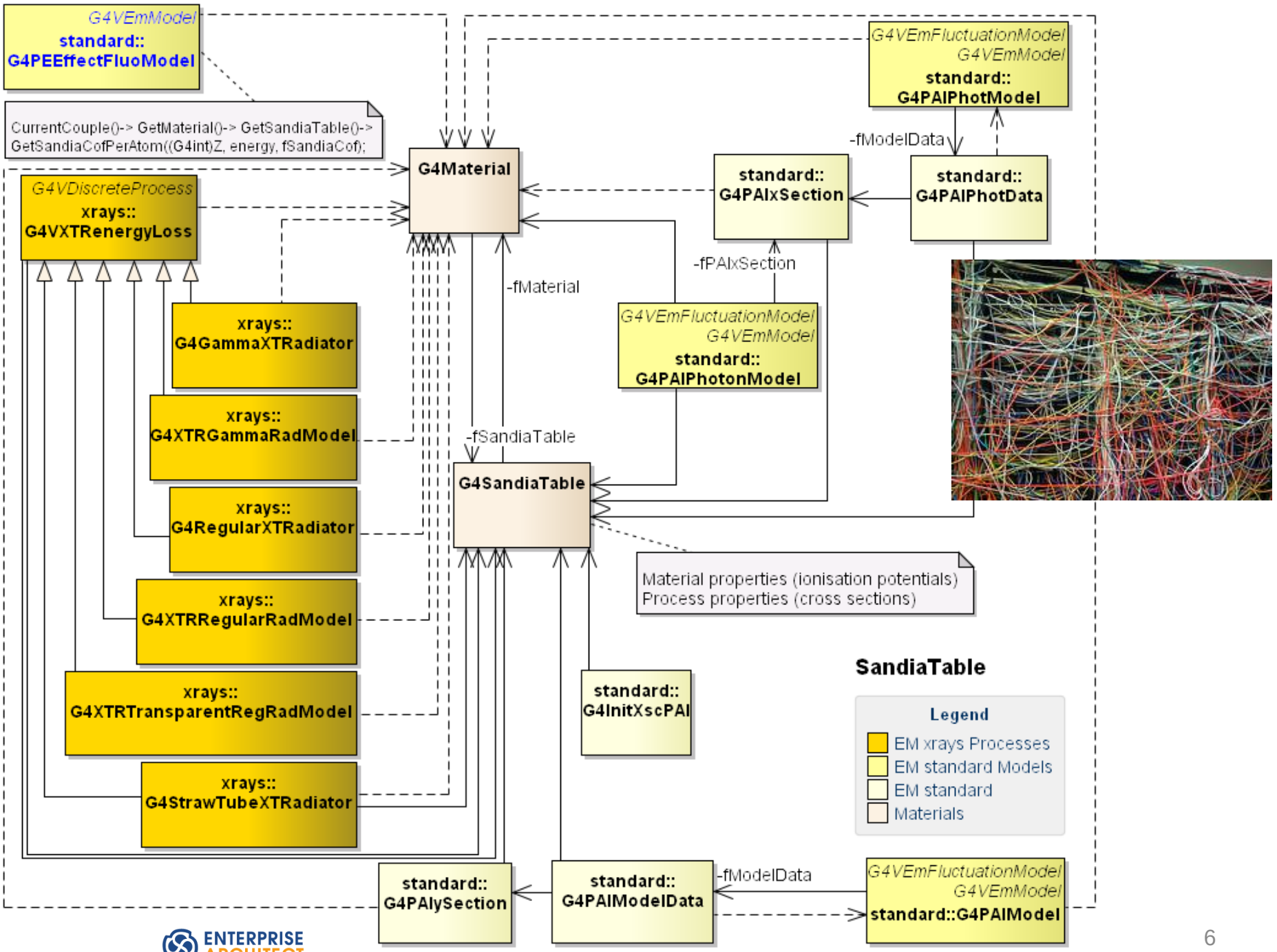
One needs a geometry
(and a full scale application)
to test any photon cross section

Difficult to test ➔ *no testing*
often

Reverse engineered

Do UML diagrams exist? Are they maintained? Peer reviews?

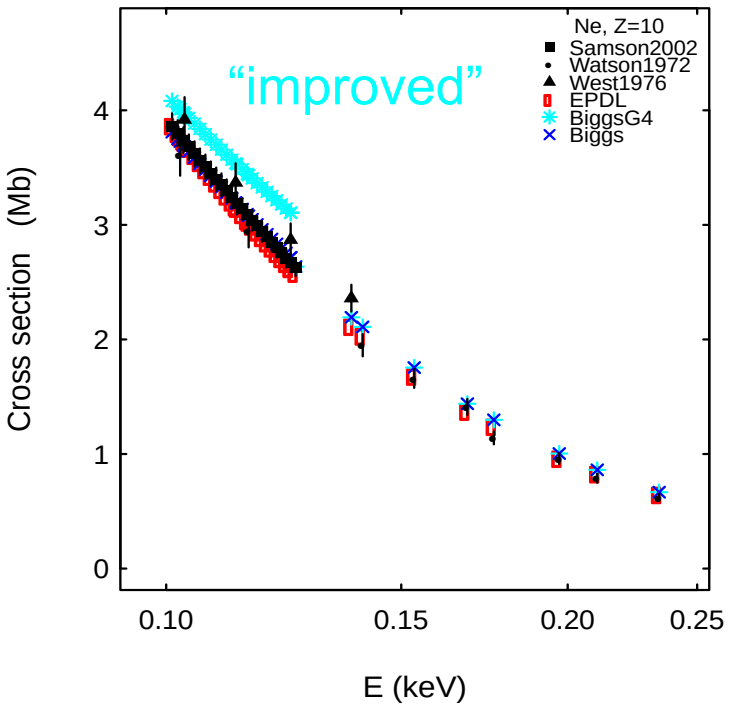
Maria Grazia Pia, *INFN Genova*

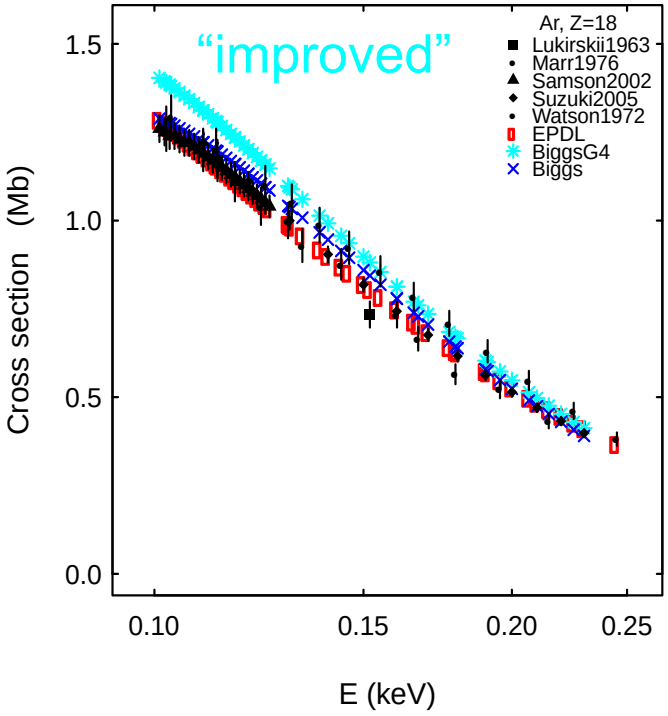

G4VEmModel
standard::
G4PEEffectFluoModel
CurrentCouple()-> GetMaterial()-> GetSandiaTable()->
GetSandiaCofPerAtom((G4int)Z, energy, fSandiaCof);
G4VDiscreteProcess
xrays::
G4VXTRenergyLoss
G4Material
G4VEmFluctuationModel
G4VEmModel
standard::
G4PAIPhotModel
-fModelData
standard::
G4PAIxSection
standard::
G4PAIPhotData
-fPAIxSection
-fMaterial
G4VEmFluctuationModel
G4VEmModel
standard::
G4PAIPhotonModel
xrays::
G4GammaXTRadiator
xrays::
G4XTRGammaRadModel
-fSandiaTable
G4SandiaTable
xrays::
G4RegularXTRadiator
xrays::
G4XTRRegularRadModel
Material properties (ionisation potentials)
Process properties (cross sections)
xrays::
G4XTRTransparentRegRadModel
standard::
G4InitXscPAI
SandiaTable
Legend
EM xrays Processes
EM standard Models
EM standard
Materials
xrays::
G4StrawTubeXTRadiator
standard::
G4PAIySection
standard::
G4PAIModelData
-fModelData
G4VEmFluctuationModel
G4VEmModel
standard::G4PAIModel

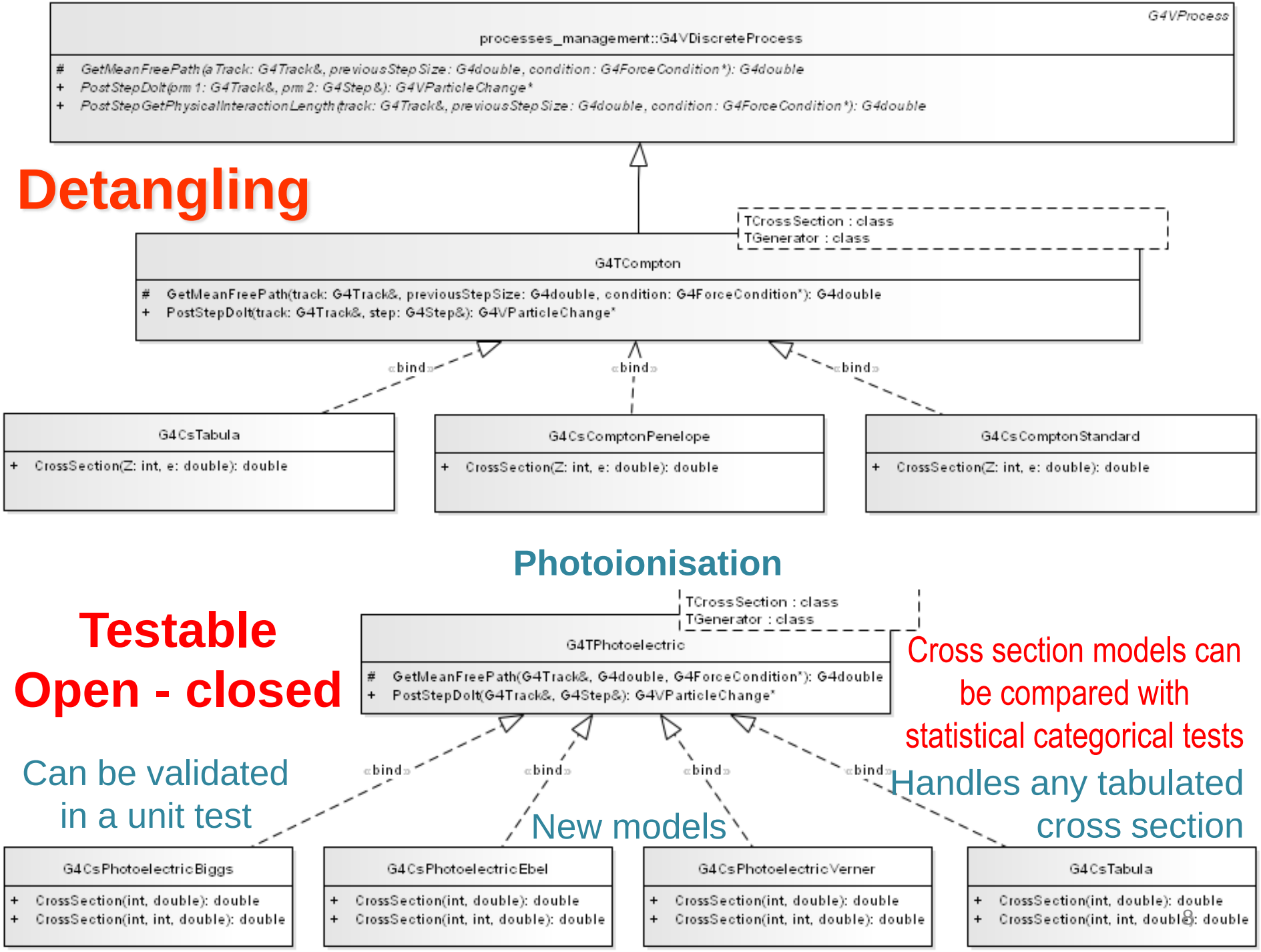
Photoionisation cross section

Cross sections in Geant4 “standard” photoelectric model are based on “**improved**” Biggs-Lighthill parameterisation

F. Biggs and R. Lighthill, Analytical Approximation for X-ray Cross Sections III, Sandia Lab. Report SAND-0070, 1988






G4VProcess
processes_management::G4VDiscreteProcess
GetMeanFreePath(aTrack: G4Track&, previousStepSize: G4double, condition: G4ForceCondition*): G4double
+ PostStepDoIt(prm1: G4Track&, prm2: G4Step&): G4VParticleChange*
+ PostStepGetPhysicalInteractionLength(track: G4Track&, previousStepSize: G4double, condition: G4ForceCondition*): G4double
Detangling
TCrossSection : class
TGenerator : class
G4TCompton
GetMeanFreePath(track: G4Track&, previousStepSize: G4double, condition: G4ForceCondition*): G4double
+ PostStepDoIt(track: G4Track&, step: G4Step&): G4VParticleChange*
«bind»
«bind»
«bind»
G4CsTabula
+ CrossSection(Z: int, e: double): double
G4CsComptonPenelope
+ CrossSection(Z: int, e: double): double
G4CsComptonStandard
+ CrossSection(Z: int, e: double): double
Photoionisation
Testable
Open - closed
TCrossSection : class
TGenerator : class
G4TPhotoelectric
GetMeanFreePath(G4Track&, G4double, G4ForceCondition*): G4double
+ PostStepDoIt(G4Track&, G4Step&): G4VParticleChange*
Cross section models can be compared with statistical categorical tests
Can be validated in a unit test
«bind»
«bind»
«bind»
«bind»
New models
Handles any tabulated cross section
G4CsPhotoelectricBiggs
+ CrossSection(int, double): double
+ CrossSection(int, int, double): double
G4CsPhotoelectricEbel
+ CrossSection(int, double): double
+ CrossSection(int, int, double): double
G4CsPhotoelectricVerner
+ CrossSection(int, double): double
+ CrossSection(int, int, double): double
G4CsTabula
+ CrossSection(int, double): double
+ CrossSection(int, int, double): double

Lehman laws

M. M. Lehman,
Programs, Life Cycles, and Laws of Software Evolution,
Proc. IEEE, vol. 68, no. 9, Sep. 1980

1. Continuing Change

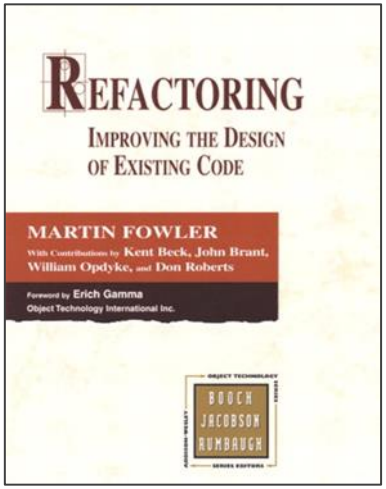
- A program that is used and that as an implementation of its specification reflects some other reality, **undergoes continual change** or **becomes progressively less useful**. The change or decay process continues until it is judged more cost effective to replace the system with a recreated version.

1. Increasing Complexity

- As an evolving program is continually changed, **its complexity**, *reflecting deteriorating structure*, **increases** unless work is done to maintain or reduce it.

Refactoring

is a disciplined technique for improving the design of an existing code

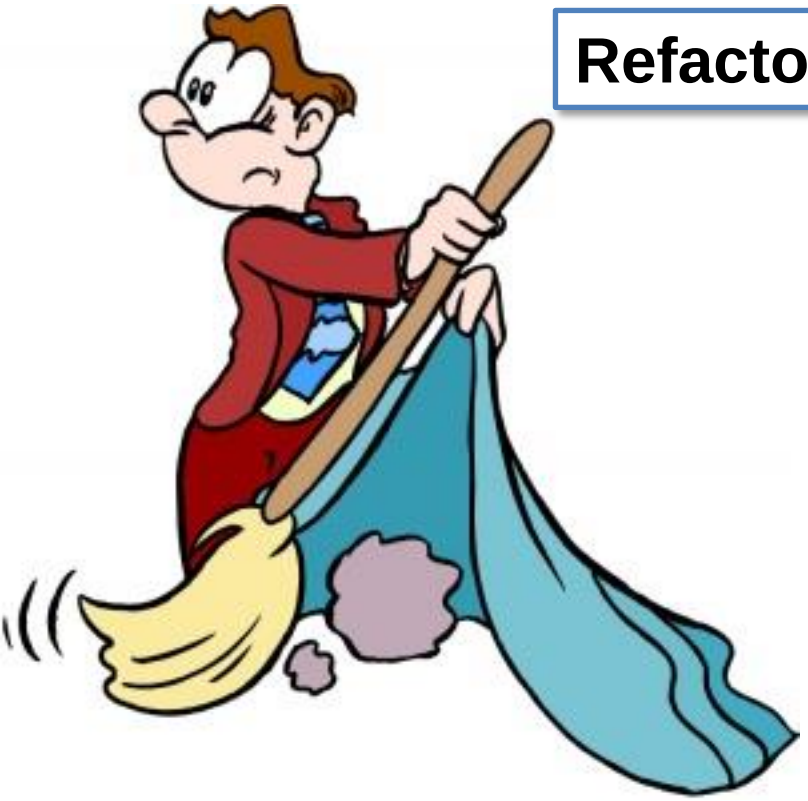


"**Refactoring** is the process of *changing* a software system in such a way that it does not alter the *external behavior* of the code yet improves its internal structure."

Refactoring begins by designing a **solid set of tests** for the portion of code under analysis

Is this all what we need?

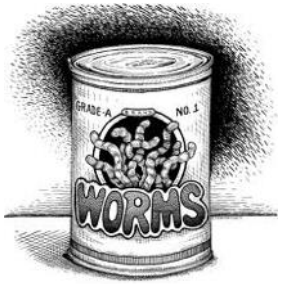
Sweeping under the carpet?



Refactoring aims to preserve correctness

Was the original code verified?

Was the original code **validated**?



IEEE Standard 1012
Software Verification & Validation
ISO 12207

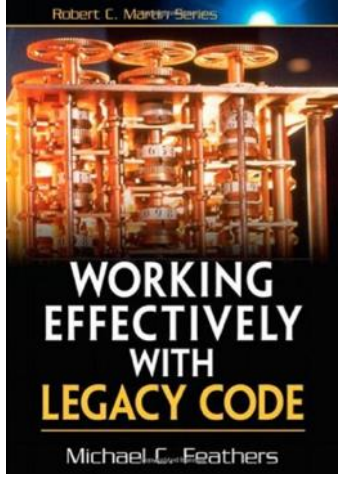
What was the test coverage?

Were the test process and the test results documented?

By improving the design, **refactoring can make software testable**

Testing à la Feather

Legacy code often lacks tests



Techniques to make existing code testable

1. Identify **change points**
2. Find an **inflection point**
3. Cover the inflection point
   a. Break external dependencies
   b. Break internal dependencies
   c. Write tests
4. Make changes
5. Refactor the covered code

can't get this class in a test harness

A narrow interface to a set of classes

If anyone changes any of the classes behind an inflection point, the change is either detectable at the inflection point, or inconsequential in the application

If the class we want to cover creates its own objects internally

Techniques to deal with irritating parameters, hidden dependencies etc.

Feasible, but painful…

Discipline of software engineering

- Most of these problems can be easily solved if we simply write tests as we develop our code
  - …and we **maintain** the tests
  - …and we **regularly execute** them
  - …and we **investigate** the reasons for failure

If a test is hard to write, that means that we have to find a different design which is testable

- It is always possible
- **Software design reviews**: care about testability

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Answer to the Ultimate Question of Life, the Universe, and Everything

Douglas Adams, The Hitchhiker's Guide to the Galaxy

// G4HadronElastic
// 29 June 2009 **(redesign old elastic model)**

```
G4double dd = 10.;
G4Pow* g4pow = G4Pow::GetInstance();
if (A <= 62) {
bb = 14.5*g4pow->Z23(A);
aa = g4pow->powZ(A, 1.63)/bb;
cc = 1.4*g4pow->Z13(A)/dd;
} else {
bb = 60.*g4pow->Z13(A);
aa = g4pow->powZ(A, 1.33)/bb;
cc = 0.4*g4pow->powZ(A, 0.4)/dd;
}
```

Testable?
Calibrated?
Epistemic uncertainties?

G4ChipsAntiBaryonElasticXS

```
lastPAR[43]=920.+03*a8*a3;
lastPAR[44]=93.+.0023*a12;
```

G4GoudsmitSaundersonMscModel

```
if(i>=19)ws=cos(sqrtA);
```

Epistemology!

G4EmCorrections

```
if(15 >= iz) {
if(3 > j) { tet = 0.25*Z2*(1.0 + 5*Z2*alpha2/16.); }
else      { tet = 0.25*Z2*(1.0 + Z2*alpha2/16.); }
}
```

G4UrbanMscModel

```
coeffc1  = 2.3785 - Z13*(4.1981e-1 - Z13*6.3100e-2);
```

Conclusion

> "Our lives begin to end the day we become silent about things that matter."
>
> *Martin Luther King, Jr.*

- Detector design, experimental strategies, physics results depend critically on software
- …which is often untested *(partially tested)* because it is untestable
  - Or became untestable in the course of its evolution
- **Making software testable**
  - Improving software design *(refactoring)*
  - Breaking dependencies *(techniques à la Feathers)*
  - **Embedding testability in the software design**
- Testability must be **maintained**
- **Epistemological** issues: domain knowledge and implementation details

Ongoing effort to make Geant4 physics testable and to test it

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