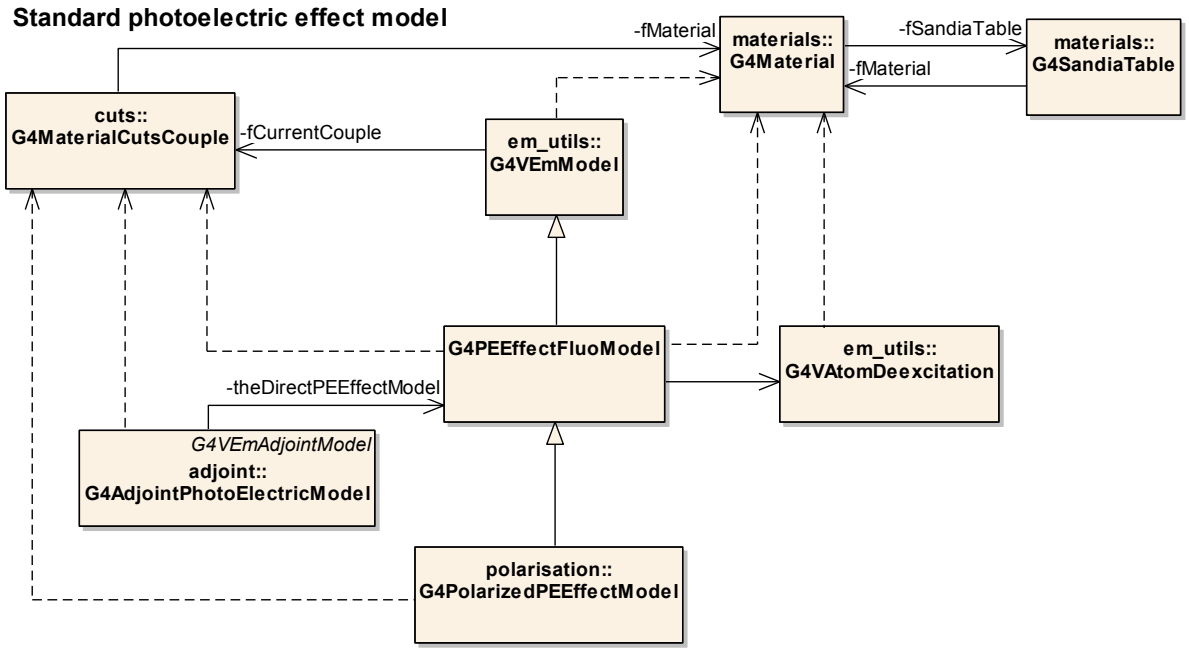


Refactoring- Exercise 2

Maria Grazia Pia

INFN Genova, Italy

Maria.Grazia.Pia@cern.ch

http://www.ge.infn.it/geant4/training/APC2014/

Simplified version of the refactoring actually done in an ongoing project of **Geant4 physics validation**

The full set of **validation results enabled by the refactoring** will be documented in a forthcoming **journal publication**

Exercise 2

A real-life physics scenario

Working with legacy code

Refactoring techniques

Guaranteed fun…

Photoelectric effect in Geant4 standard electromagnetic package

Photoelectric cross section based on an empirical formula:

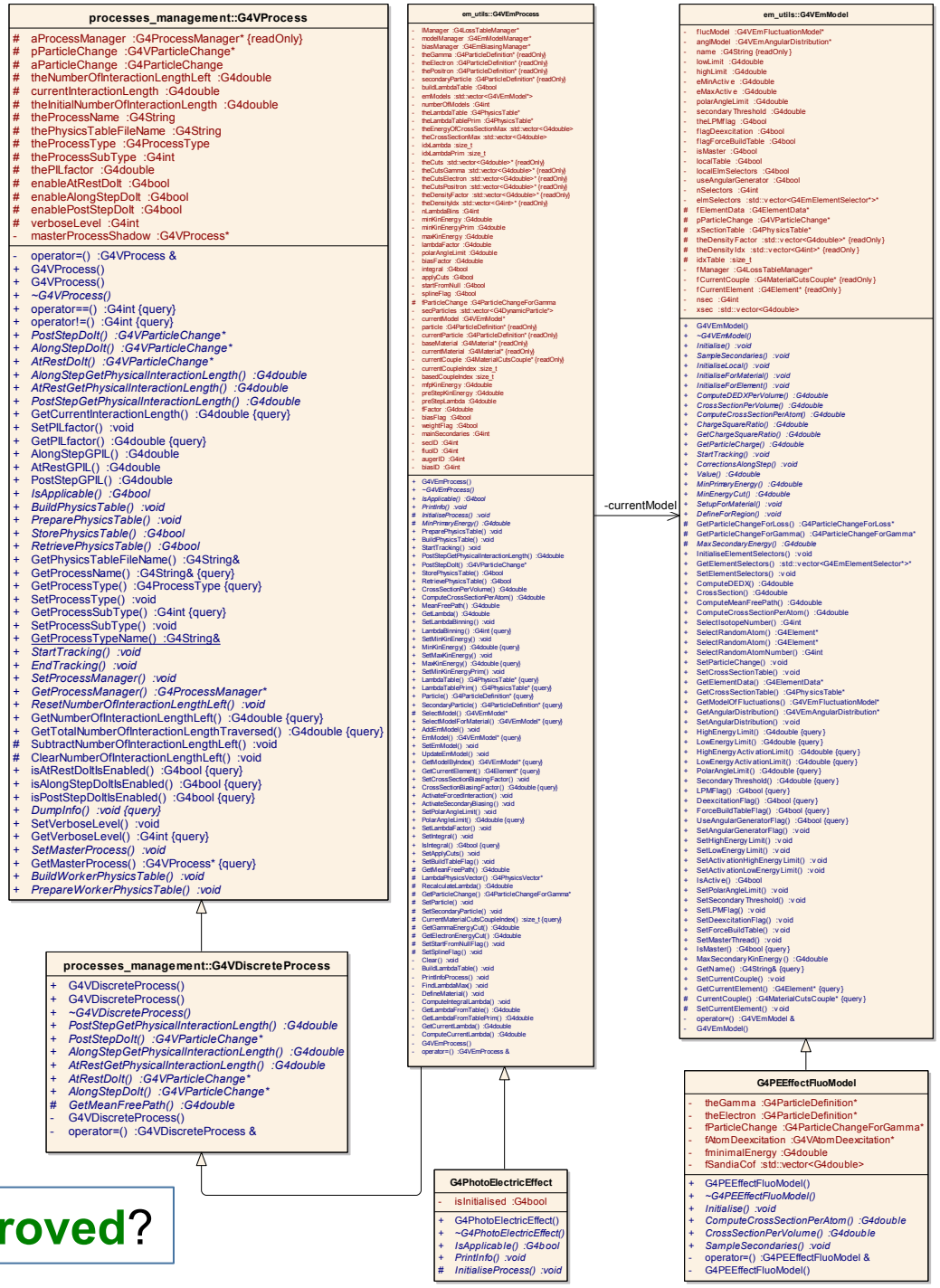
$$\mu_{ij} = \frac{A_{ij1}}{E} + \frac{A_{ij2}}{E^2} + \frac{A_{ij3}}{E^3} + \frac{A_{ij4}}{E^4}$$

F. Biggs and R. Lighthill, Analytical Approximations for X-Ray CrossSections III, Sandia Report SAND87-0070, 1988

For some elements and intervals Geant4 uses A_{ij} parameters **improved** over the *original* A_{ij}

We want to **validate** Geant4 standard photoelectric cross section w.r.t. experimental data

How much has the accuracy **improved**?



Prepare the material for the exercise

- Download the tarball: `wget` http://www.ge.infn.it/geant4/training/APC2014/exercise2/APC2014ex2.tgz
- Unpack the tarball in your home directory: `tar -zxf APC2014ex2.tgz`
- In $HOME/*APC2014ex2:*

geant4.10.00.p01	Geant4 code, version 10.0-patch01
work10APC	Geant4 libraries and test executables
parametersAPC	original" and "improved" A_{ij} parameters
dataAPC	experimental data for validation
test	test code for the refactoring process
rwork	R scripts for data analysis
setup10APC.csh, setup10APC.sh	

- Define environment variables for the exercise: `source setup10APC.csh` *`(or setup10APC.sh)`*

Solutions

- Solutions corresponding to the various phases of the exercise can be downloaded from http://www.ge.infn.it/geant4/training/APC2014/exercise2.html
- Beware: although simplified for the APC school, this is still unpublished material, which is intended to go into a publication
- Two students Min Cheol Han, Han Sung Kim (Hanyang Univ., Seoul) contributed significantly to Geant4 photoelectric effect refactoring and validation

Photoelectric cross section

G4PEEffectFluoModel

$G4INSTALL/source/processes/electromagnetic/standard/includeG4PEEffectFluoModel.hh
$G4INSTALL/source/processes/electromagnetic/standard/src/G4PEEffectFluoModel.cc

G4PEEffectFluoModel has a member function

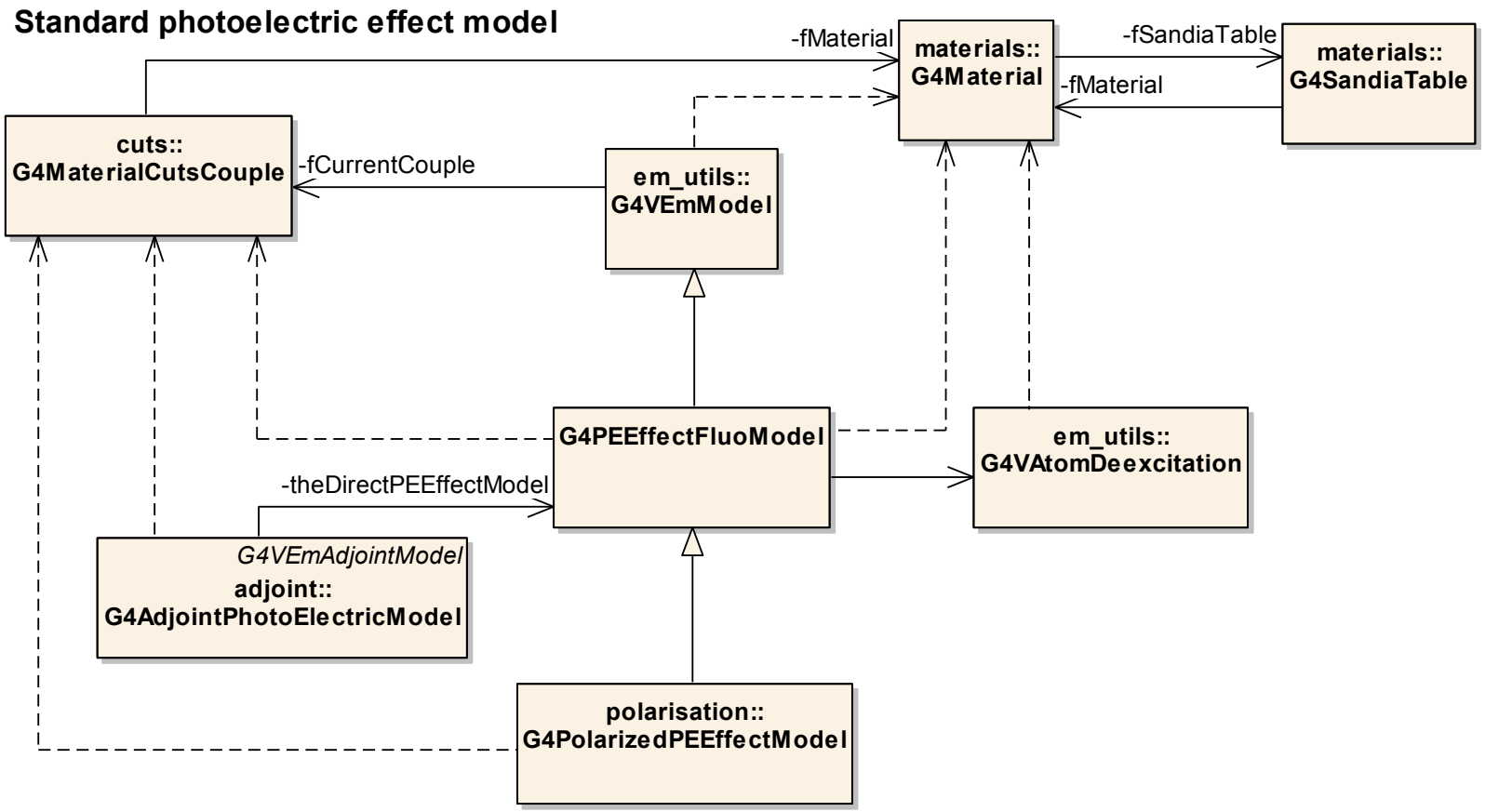
```
G4double ComputeCrossSectionPerAtom(const G4ParticleDefinition*,
                                    G4double kinEnergy,
                                    G4double Z,
                                    G4double A,
                                    G4double, G4double)
```

This is what we are looking for indeed!

Testing G4PEEffectFluoModel cross section

- Create a simple *G4PEEffectFluoModelTest.cc*, which
  - instantiates a *G4PEEffectFluoModel* object
  - invokes *ComputeCrossSectionPerAtom*
  - Calculates pre-defined configurations of photon energy and target element
- Place the unit test in $APCDIR/test
- **Build the test**:
  cd $APCDIR/test
  setenv TESTTARGET G4PEEffectFluoModelTest
  gmake
- **Run the test**:
  $G4WORKDIR/bin/Linux-g++/G4PEEffectFluoModelTest
- **Translate the result into Bavarian**

Hidden dependencies

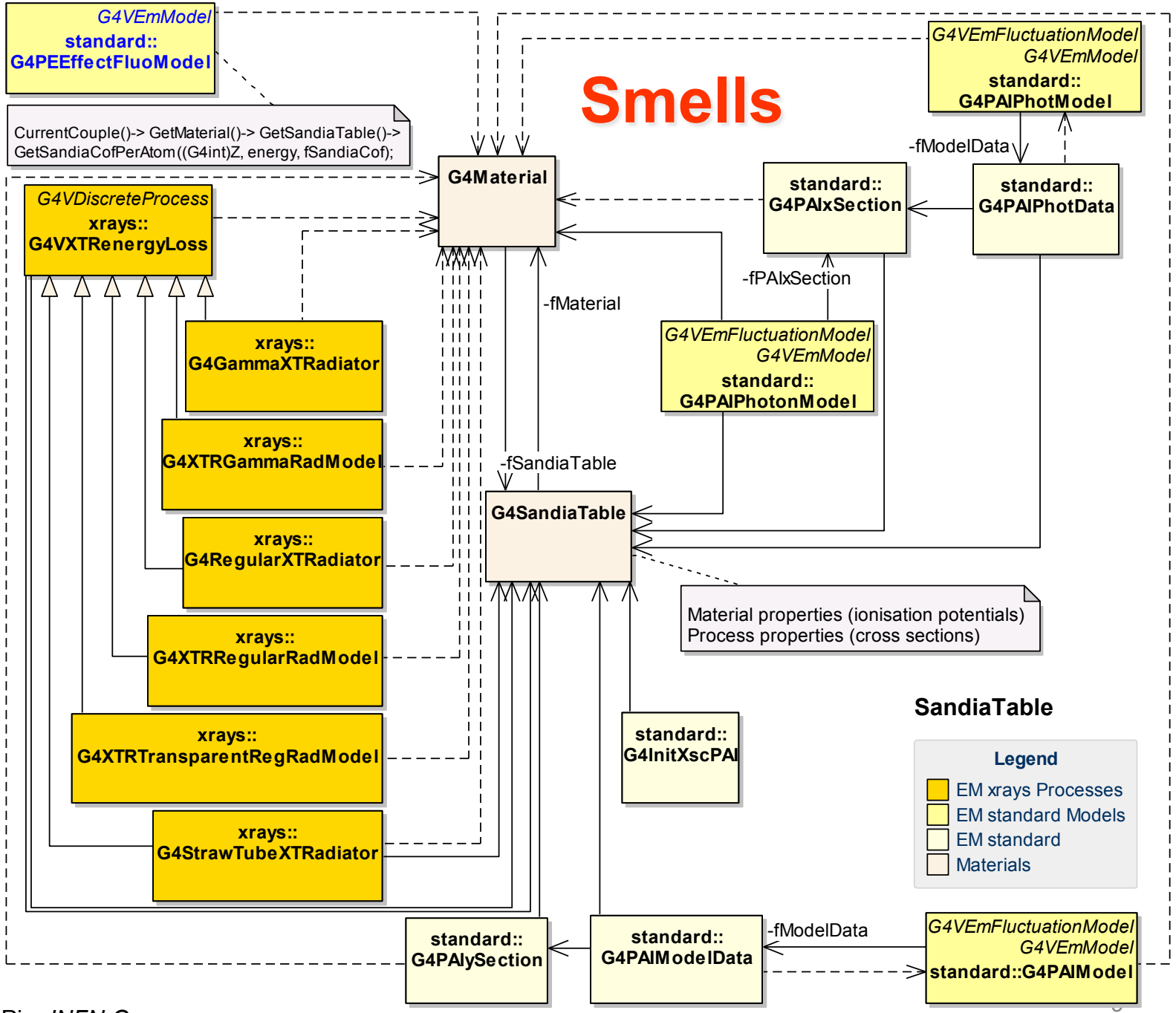


M. Feathers, "Working Effectively with Legacy Code"

Techniques to make the calculation of the photoelectric cross section

testable

Smells


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

Identify smells

- Long argument list of *ComputeCrossSsectionPerAtom* smells of **Speculative Generality**
- *G4SandiaTable* is a **Large Class** with fuzzy responsibility
  - (what is the relation between calculating photoelectric cross sections and ionization potentials?)...
- *etc.*

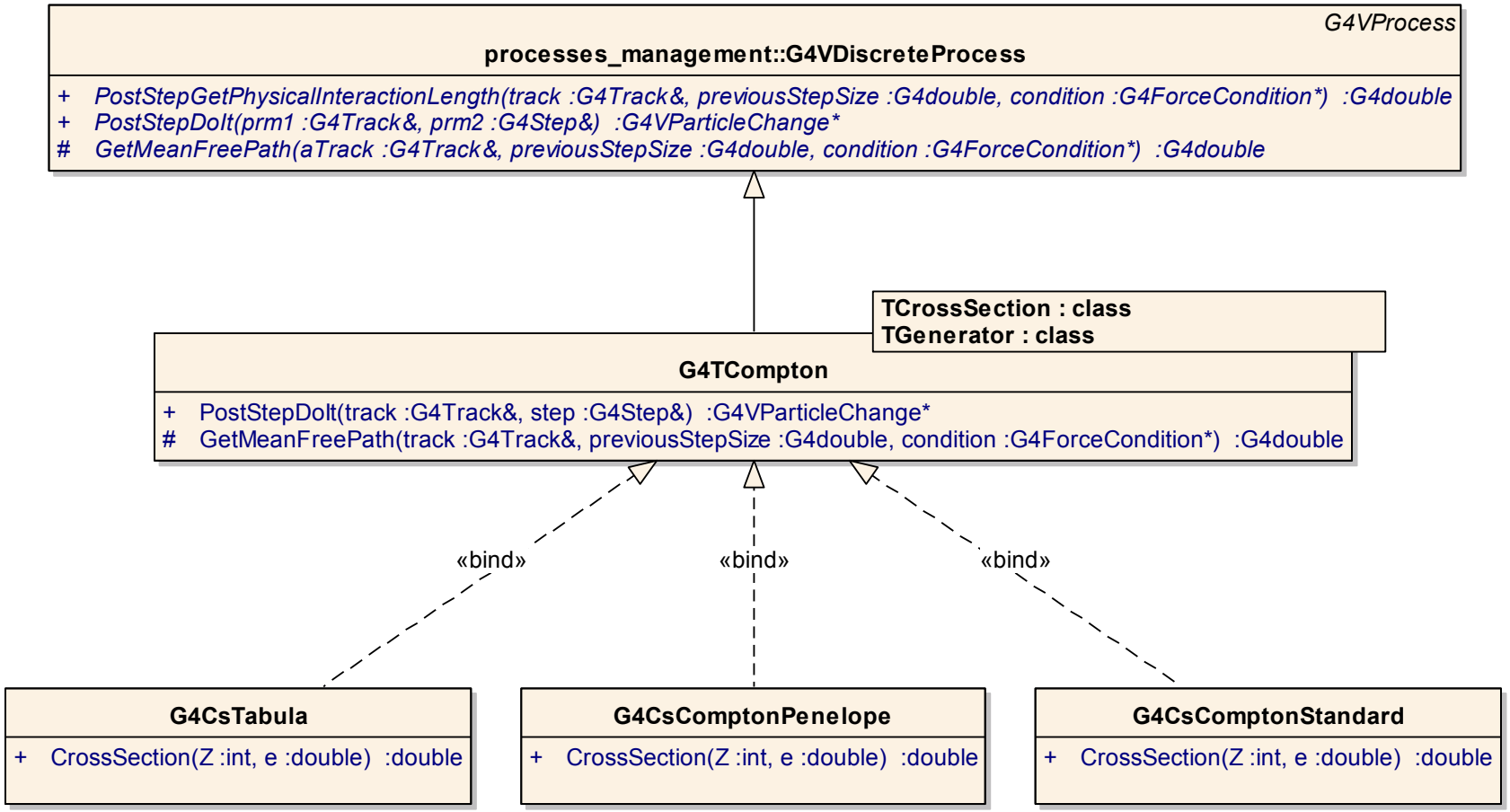
- Hunt for more smells!
- List of smells
  http://www.industriallogic.com/wp-content/uploads/2005/09/smellstorefactorings.pdf

Physicist's attitude

- As physicists, we want to be able to know the cross sections used in our simulation and to compare them with experimental data without creating unnecessary objects that have no relation with a cross section.
- **Refactor** (reengineer) the code and make the photoelectric cross section **testable**
- Apply **Extract Class**
- Create a new *G4CsPhotoelectricAPC* class
- Move the relevant fields and methods from the old *G4SandiaTable*, *G4StaticSandiaData and G4PEEffectFluoModel* classes into the new class
- **Hint:** G4CsComptonAPC class in $G4INSTALL/*source/processes/electromagnetic/pii/*
  - simplified version of the actual class that will be documented in the forthcoming publication

How could a testable cross section class fit into Geant4

(Simplified) hint about introducing a testable cross section class in Geant4 kernel design



Compiling new or modified classes

- Place new classes in
  $G4INSTALL/source/processes/electromagnetic/pii/
  `pii/include/G4CsPhotoelectricAPC.hh` (header file)
  `pii/src/G4CsPhotoelectricAPC.cc` (implementation)

- Whenever you add or modify a class in the pii package, recompile it:
  ```
  cd $G4INSTALL/source/processes/electromagnetic/pii/
  gmake
  ```

- The resulting library will be in $G4LIB/Linux-g++/libG4empii.a
- Then build (or rebuild) the corresponding unit test as previously shown

Testing the new class

- Create a test for *G4CsPhotoelectricAPC* class in *$APCDIR/PhotoelectricAPCTest.cc*
- Hint: a test for the similar Compton cross section class in http://www.ge.infn.it/geant4/training/APC2014/code2/test/ComptonAPCTest.cc
- Build and run the test:
  cd $APCDIR/test
  setenv TESTTARGET PhotoelectricAPCTest
  gmake
  $G4WORKDIR/bin/Linux-g++/PhotoelectricAPCTest
- How do we verify that *G4CsPhotoelectricAPC* is **correct** and **equivalent** to the cross section calculation in *G4PEEffectFluoModel*?
  - *G4PEEffectFluoModelTest* does not let us test cross sections
  - Compare with the reference plots in the Sandia87-0070
  - Shortcut for the APC some previously verified reference values in http://www.ge.infn.it/geant4/training/APC2014/exercise2/dataAPC/all_photoelectricAPC.txt
    - column 6: cross sections with original A_{ij} parameters
    - column 7: cross sections with improved parameters

Adding functionality to the new class

- How much did the **improved parameters** actually improve the accuracy of photoelectric cross sections?
- We require the capability to calculate cross sections with **original** or **improved** A_{ij} parameters
  - In *G4PEEffectFluoModel* this is not possible, since the parameters are hardcoded in *G4StaticSandiaData*
- Hint: store the parameters in external files and make *G4PhotoelectricAPC* load them when it is instantiated
- For your convenience, files containing the two sets of original and improved A_{ij} parameters are available in *$APCDIR/parametersAPC/*
- You may pass an argument to the constructor of *G4PhotoelectricAPC* to decide whether to load the original or improved parameters

Comparison with experimental data

Experimental data

$APCDIR/data/exp_photoelectricAPC.txt

Columns:

1. Published reference identifier
2. Z
3. Energy (keV)
4. Cross section (b)
5. Cross section error (b)

Your test should produce

$APCDIR/data/all_photoelectricAPC.txt

Columns:

1. Published reference identifier
2. Z
3. Energy (keV)
4. Cross section (b)
5. Cross section error (b)
6. Cross section (b) calculated with original A_{ij} parameters
7. Cross section (b) calculated with improved A_{ij} parameters

Plot photoelectric cross sections with R

- No-frills basic R environment for this simple analysis
  - no GUI, only R core packages, basic graphics etc.
  - you can do much more with a powerful system such as R!
- *$APCDIR/rwork/plotAPC.R* plots experimental and calculated photoelectric cross sections for Z=10 (neon) and Z=18 (argon)
- Start R:

```
cd $APCDIR/rwork
R -g Tk &
```

- In the R console click on the File menu on the top left corner, choose "Source R code" and select the plotAPC.R script
  - will load the file *$APCDIR/dataAPC/all_photoelectricAPC.txt*
  - will produce the plots in the R graphics window
  - will place a copy in PDF files in the same directory