



Physics methods for the simulation of photoionisation

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"Beyond Imagination of Future Science"

Rationale

Simulation physics

The simulation of photon physics is well-established.

→ Is there any quantitative validation?

New physics

New theoretical calculations and parameterisations were released recently.

→ Are they accurate than old one?

New trends

Very low energy (~eV scale) & micro/nano dosimetry
ex. FLUKA, Geant4-DNA, MOCA, OREC/NOREC, PARTRAC, Penelope, PTB-code, Trion etc.

→ How accurate are models?

Project to validate **quantitatively** a wide set of simulation modeling options against a large collection of experimental data

State-of-the-art simulation of photon interactions

Elastic scattering
: **Published**

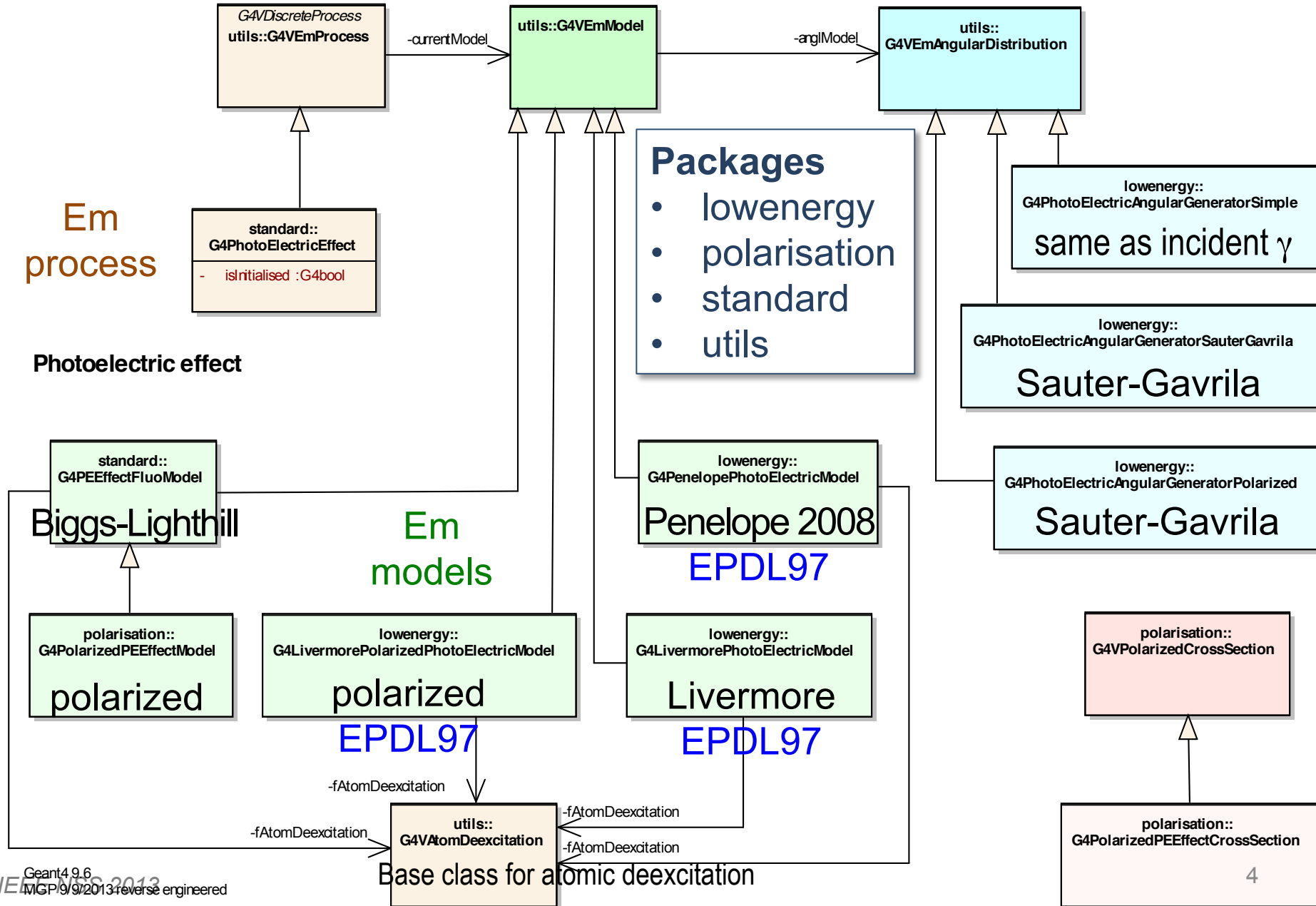
Photoelectric effect

Compton scattering
pair production
: **first results**

Photoionisation in Monte Carlo codes

	Cross sections	Angular distribution
EGS5	PHOTX	Sauter
EGSnrc	Storm-Israel Fit to XCOM EPDL97 (subshell)	Sauter
FLUKA	EPDL97	Sauter
Geant4	Revised Biggs-Lighthill (Henke) EPDL97	Sauter-Gavrila Same direction
ITS	Scofield 1973	Fischer+Sauter
MCNP(X)	EPDL89, EDPL97 ENDFB/IV+Storm-Israel	
Penelope	EPDL97	Sauter (K shell)

Photoionisation in Geant4 9.6



Cross section sources

Year	Compilation	Energy	Z	(sub)Shell	Method
1967-1988	Biggs-Lighthill	10 eV – 100 GeV	1-100	-	parameterised
1992	Brennan-Cowan	30 eV – 700 keV	3-92	-	tabulated
2000	Chantler	10 eV – 433 keV	1-92	K	tabulated
2003	Ebel	1 keV – 300 keV	1-92	all	parameterised
2002	Elam	100 eV – 1 MeV	1-98	-	tabulated
1997	EPDL97 (<i>Scofield</i>)	10 eV – 100 GeV	1-100	all	tabulated
1982-1993	Henke	10 eV – 30 keV	1-92	-	tabulated
1970-2006	McMaster/Shaltout	1 keV – 700 keV	1-94	-	tabulated
1989	PHOTX (<i>Scofield</i>)	1 keV – 100 MeV	1-100	-	tabulated
2001	RTAB	10 eV – 30 keV	1-99	all	tabulated
1973	Scofield	1 keV – 1.5 MeV	1-100	all	tabulated
1970	Storm-Israel	1 keV – 100 GeV	1-100	-	tabulated
1973	Veigele	100 eV – 100 MeV	1-94	-	tabulated
1987-2010	XCOM (<i>Scofield</i>)	1 keV – 100 GeV	1-100	-	tabulated

Different methods and calculations

e.g. Chantler's exchange potential in his DHF calculation is different from Scofield's

Strategy

- Evaluate a large number of available modeling options
- Suitable for use in Monte Carlo simulation codes
 - Tabulated theoretical calculations
 - Simple analytical formulations, with documented parameters
- All options evaluated in the same computational environment
 - Minimize dependencies on other software parts (*not always components*)
- Quantitative, objective evaluation based on **statistical methods**
- Establish state-of-the-art for the simulation of photoionisation on objective ground
- Computational performance measured along with physical accuracy

※ We only focus on the simulation with non-polarised photons case.

Computational environment

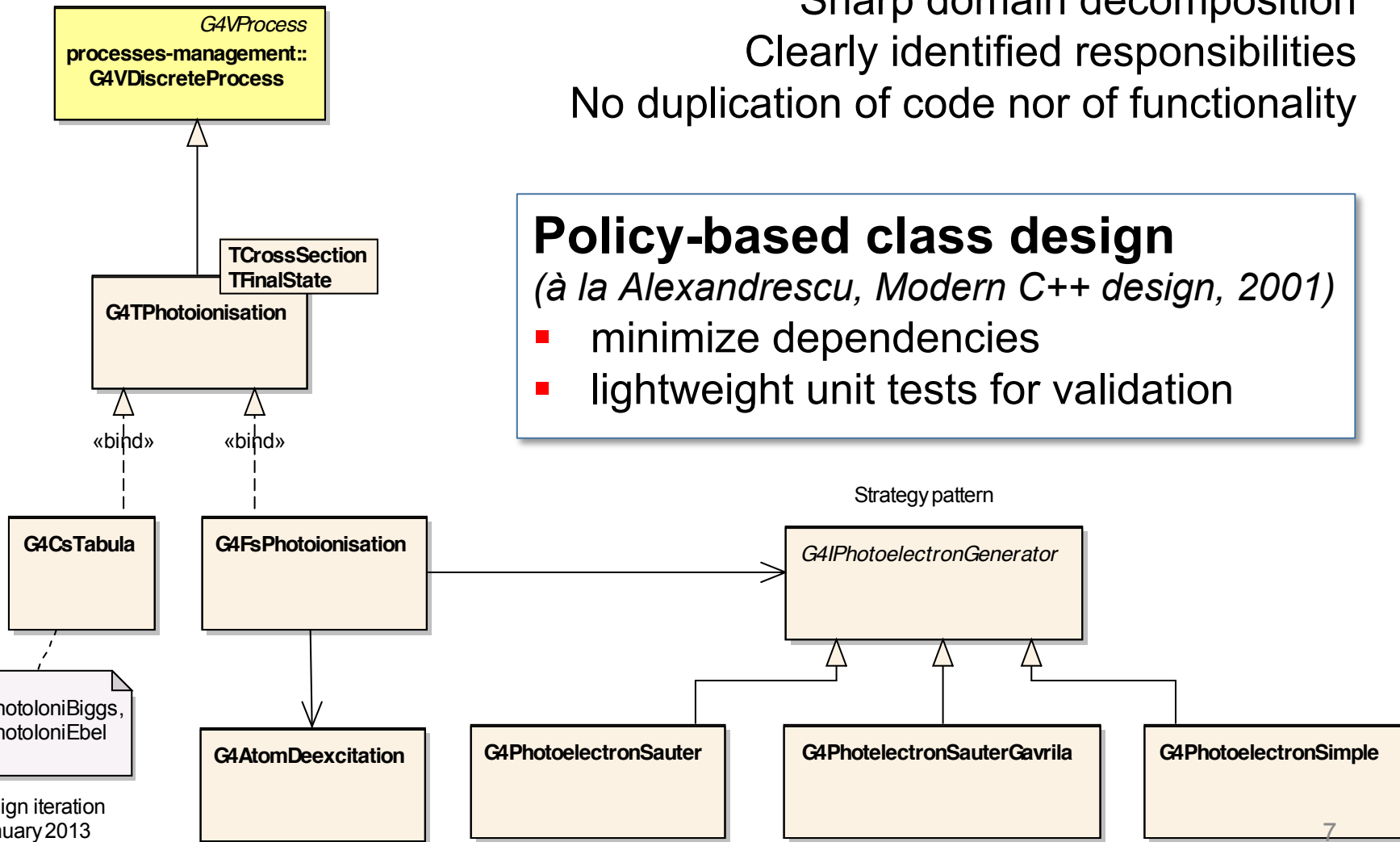
Streamlined software design consistent with Geant4 kernel

Sharp domain decomposition
Clearly identified responsibilities
No duplication of code nor of functionality

Policy-based class design

(à la Alexandrescu, *Modern C++ design*, 2001)

- minimize dependencies
- lightweight unit tests for validation



Experimental data

● Collected from the literature

- Total cross sections
- Partial cross sections
- Angular distributions

> 150 references
> 5000 data points
~ 3700 σ_{total}
~ 1400 σ_{shell}

● Data types

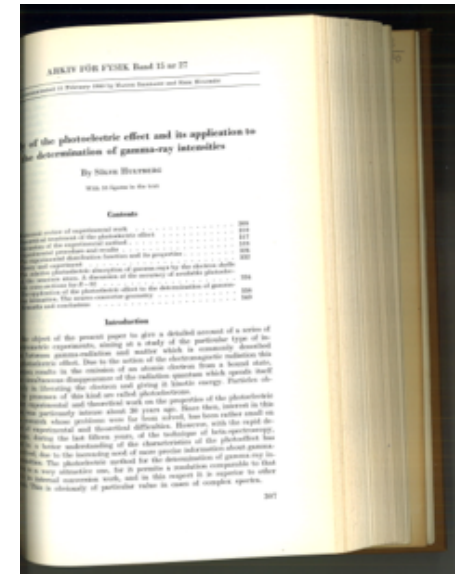
- **Pure experimental** cross sections: direct measurements
- **Semi-empirical** cross sections: involve theoretical manipulations
 - ▶ e.g. subtraction of calculated scattering contribution (Compton and elastic)

● Format

- Tables, text
- Figures: digitized, digitization error estimated

● Evaluation of experimental data

- Systematic effects: identified whenever possible
- Outliers

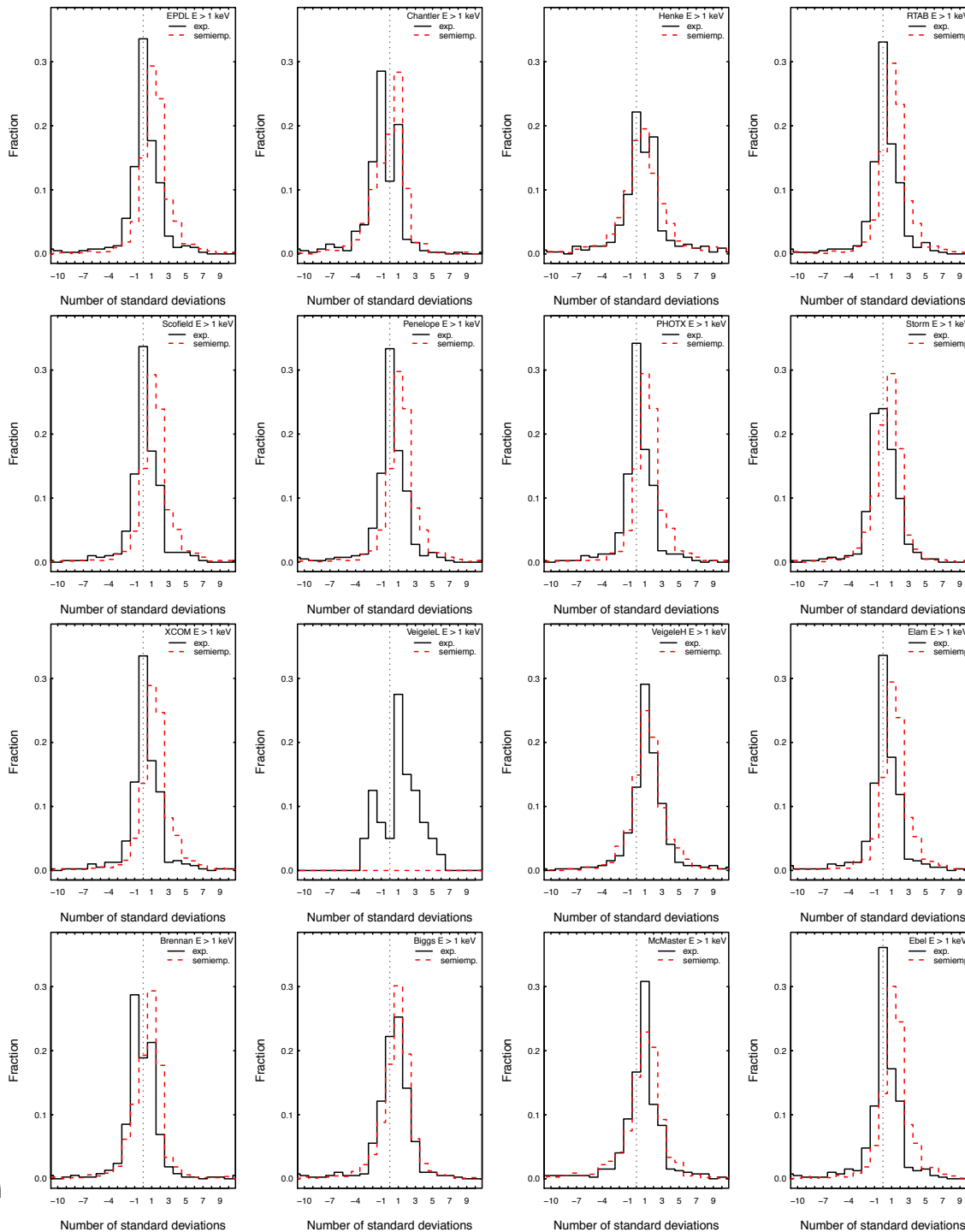


Systematic effect?

Difference between calculated and “experimental” total cross sections, expressed in terms of number of standard deviations:

pure experimental
and
semi-empirical
data

Only pure experimental data used in the validation process



Data analysis method

- Two-stage statistical analysis
 1. Compatibility of each cross section calculation method with experiment
 2. Comparison of compatibility with experiment across modeling categories
- Quantitative appraisal of capabilities and differences

Compatibility with experiment

Goodness-of-fit test

χ^2 test
 $\alpha = 0.01$

$\alpha \geq 0.01 \rightarrow$ pass

$\alpha < 0.01 \rightarrow$ fail

efficiency = $N_{\downarrow pass} / N_{\downarrow test\ cases}$

Difference across categories

Contingency tables

Fisher exact test

Barnard test

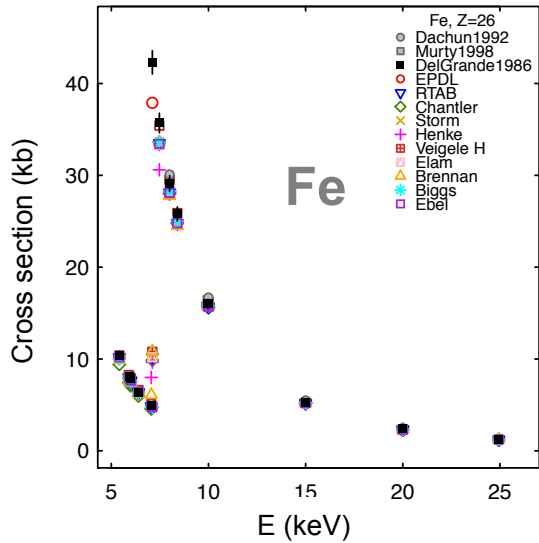
Pearson χ^2 test

$\alpha = 0.05$

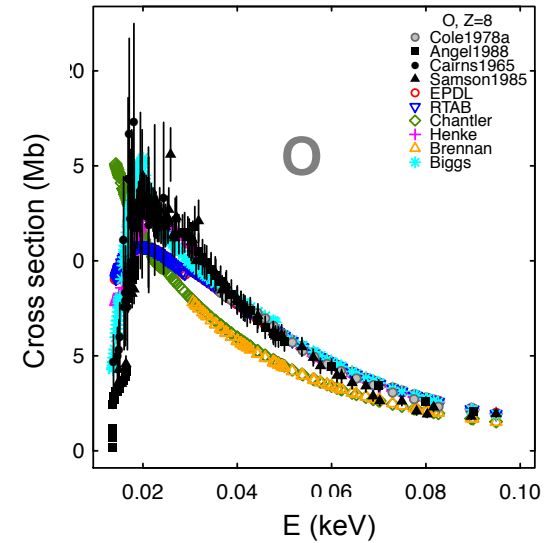
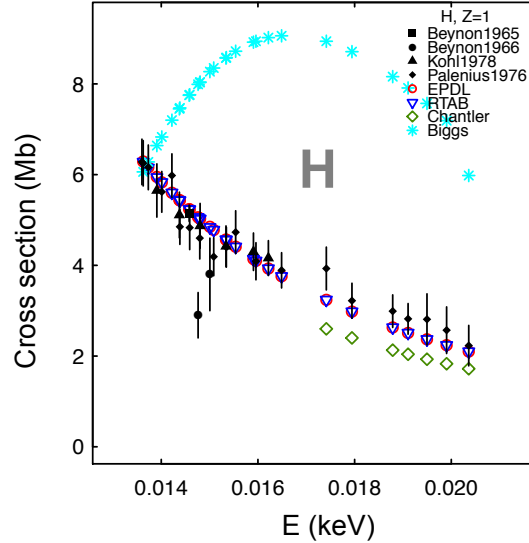
as appropriate

Results - Total cross sections

E > 250 eV



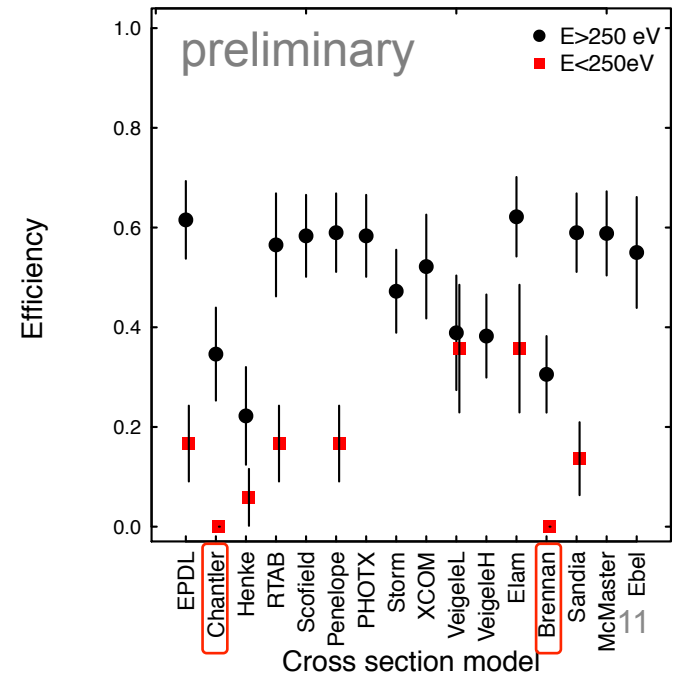
E < 250 eV



- Most calculation methods exhibit similar compatibility with experiment for **E > 250 eV**
 - Chantler, Brennan-Cowan look worse
- Degraded accuracy below 250 eV

Analysis of contingency tables

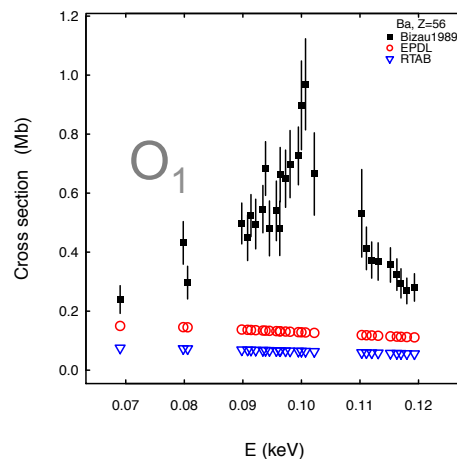
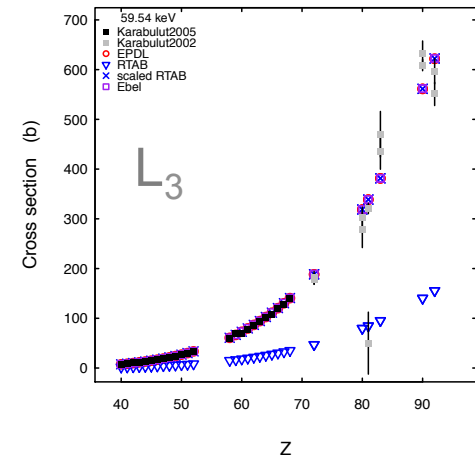
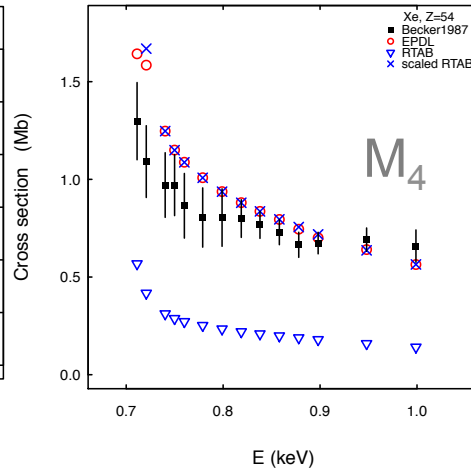
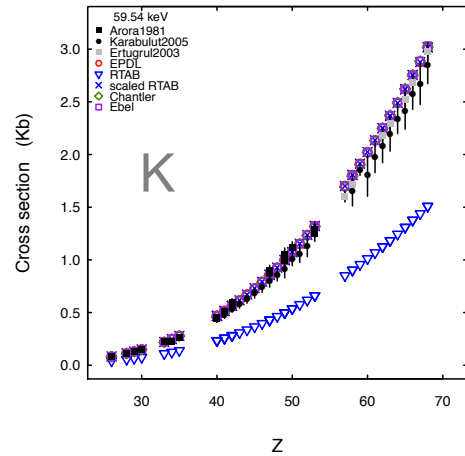
	EPDL Chantler	EPDL Brennan-Cowan
Fisher	0.044	0.011
Pearson χ^2	0.033	0.007
Barnard	0.035	0.007



Results - Shell cross sections

Calculated **inner shell** cross sections compatible with experiment

Outer shell cross sections inconsistent with experimental data
Beware: small data sample, limited data sources



p-value χ^2 test

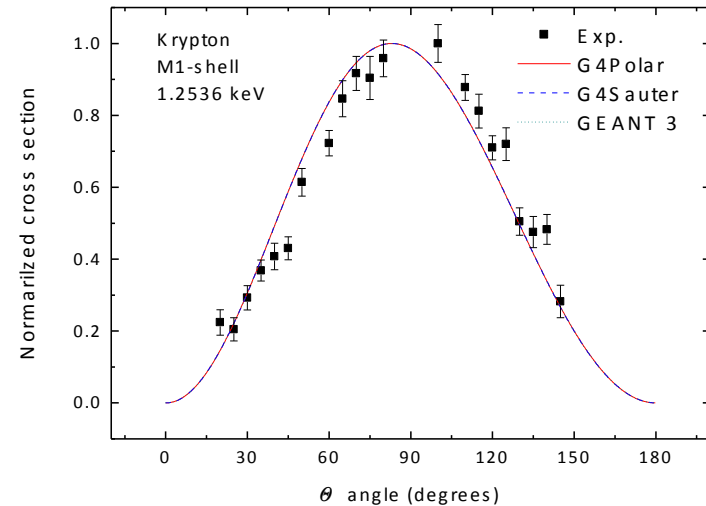
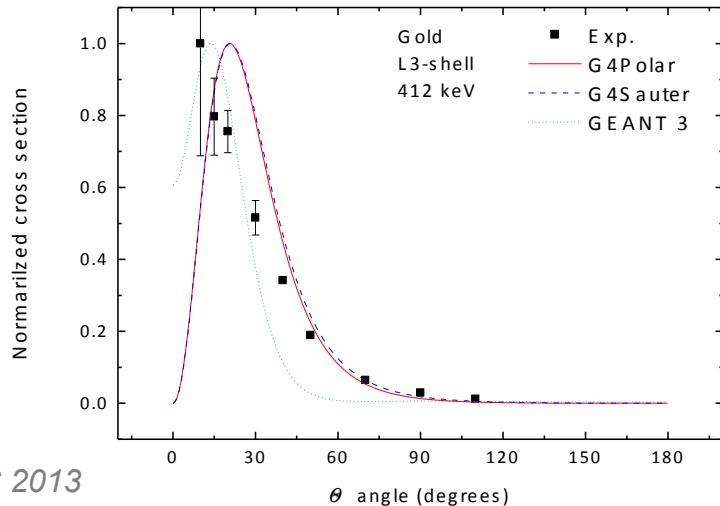
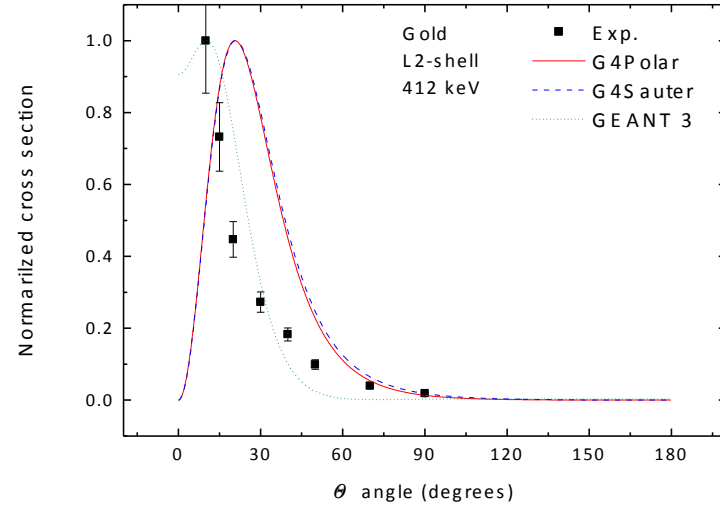
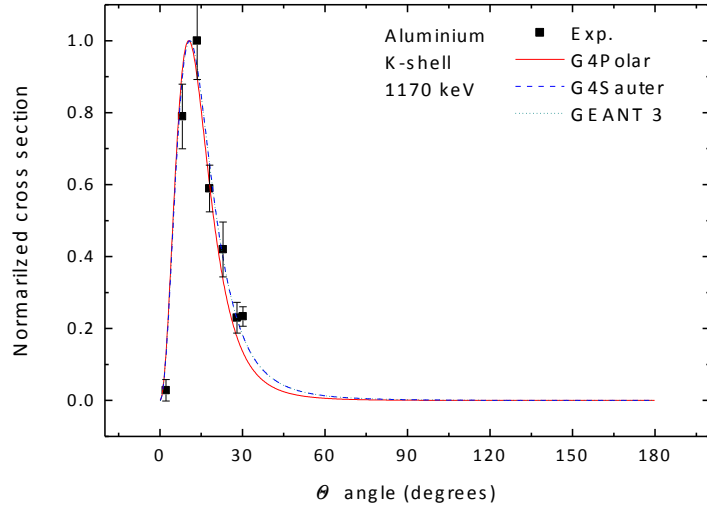
shell	EPDL	Chantler	RTAB	scRTAB	Ebel
K	0.209	0.350	<0.001	0.315	<0.001
L1	0.075		<0.001	0.069	0.964
L2	0.339		<0.001	0.299	0.154
L3	1		<0.001	1	1
M1	<0.001		<0.001	<0.001	
M4	0.031		<0.001	<0.001	
M5	<0.001		<0.001	<0.001	
N1	<0.001		<0.001	<0.001	
N6	<0.001		<0.001	<0.001	<0.001
N7	<0.001		<0.001	<0.001	<0.001
O1	<0.001		<0.001	<0.001	<0.001
O2	<0.001		<0.001	<0.001	<0.001
O3	<0.001		<0.001	<0.001	<0.001
P1	<0.001		<0.001	<0.001	<0.001

Systematic effect observed with RTAB shell cross sections (presumably a missing factor in the calculation)

Results - Angular distribution

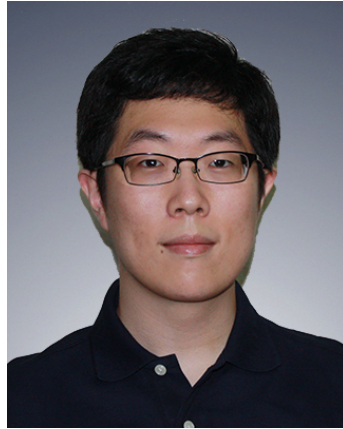
Option à la GEANT 3 (Sauter) evaluated along with other Geant4 options

Qualitative appraisal
Limited experimental sample
Experimental systematic effects
(corrected/uncorrected data)



Conclusion

- **Large scale effort to evaluate quantitatively physics methods for photoionisation simulation**
 - Part of a wider project for **quantitative** assessment of **state-of-the-art** simulation of photon interactions
- **Total cross section**
 - Most calculation methods exhibit similar behaviour
 - More recent calculations (Chantler, Brennan-Cowan) do not appear more accurate than old Scofield's 1973 (unrenormalized)
- **Inner shells**
 - EPDL, (*corrected*) RTAB appear equivalent, Ebel's parameterisation inconsistent with experimental K shell data
- **Outer shells**
 - No calculation method appears adequate to reproduce experimental data
- **Photoelectron angular distribution**
 - Scarce data and experimental systematics prevent a quantitative discrimination



...a big **THANK YOU** to
the CERN Library!