

**New Geant4 developments for Doppler broadening simulation in Compton scattering**

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**Development of Charge Transfer Simulation Models in Geant4**

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**Validation of Geant4 electromagnetic models against calorimetric measurements in the energy range up to 1 MeV**

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**Validation of Geant4 X-ray fluorescence transitions**

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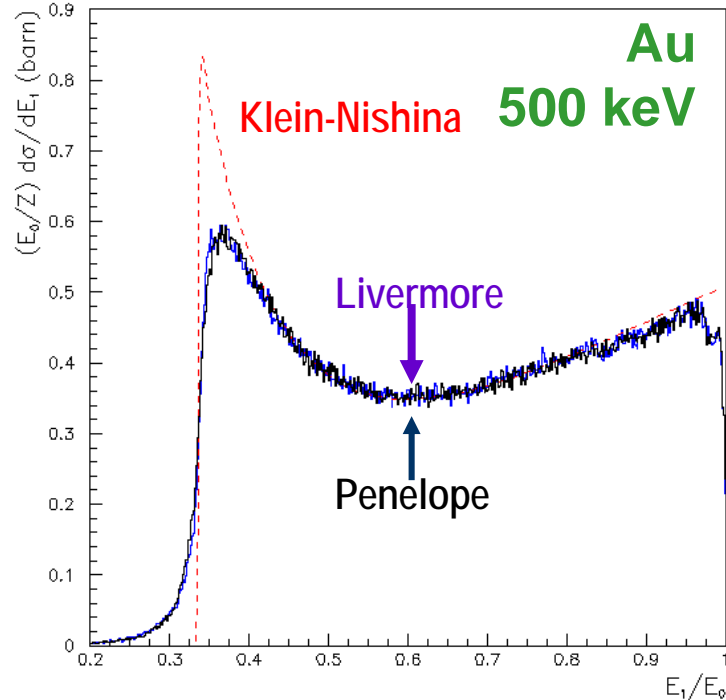
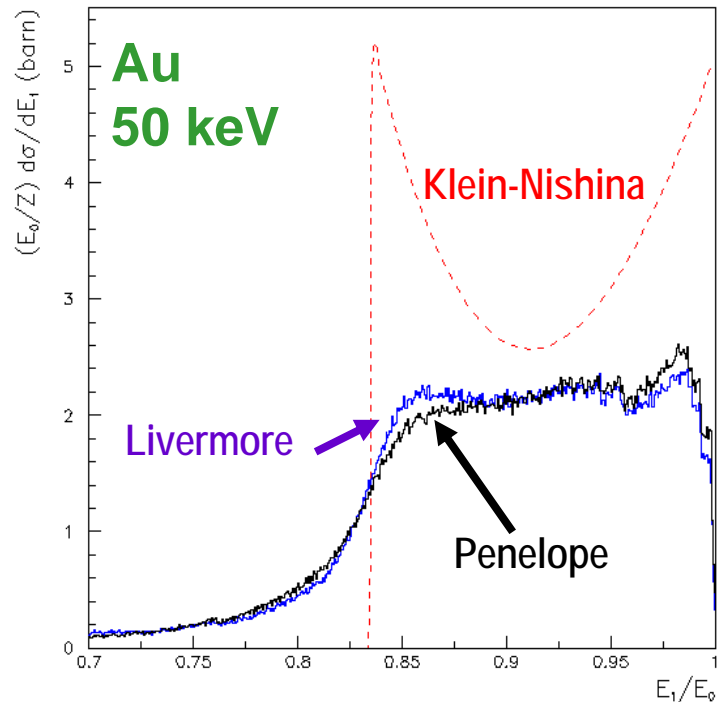
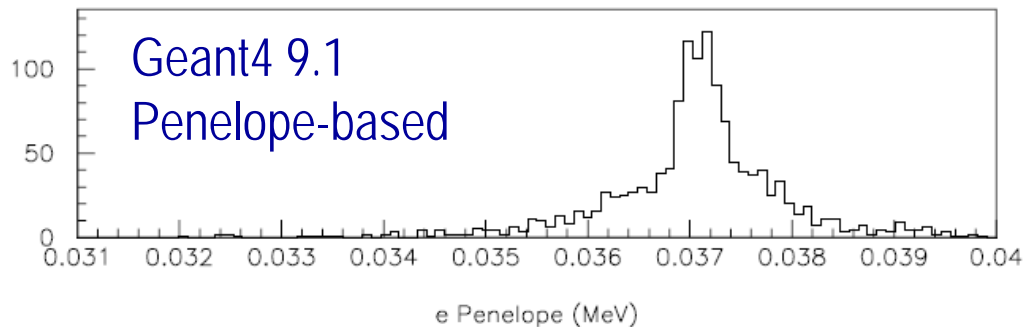
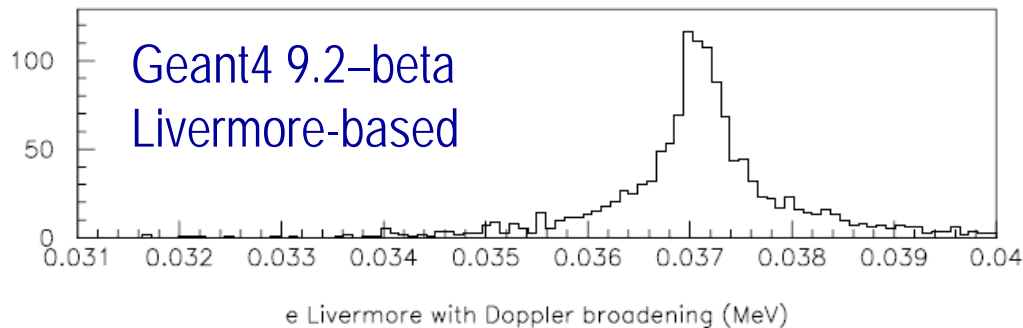
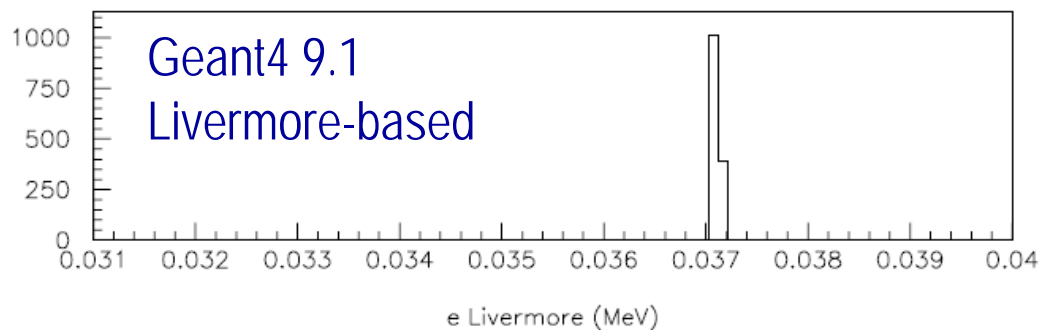
*IEEE Nuclear Science Symposium  
Dresden, 19-25 October 2008*

# Doppler broadening

- Accounts for **electron binding** effect in Compton scattering
- Fundamental limit for the angular resolution of Compton scattering-based telescopes
- Contributes to the resolution in Compton cameras in medical imaging
- **Until Geant4 9.1** Doppler broadening only in Compton scattering based on Penelope models (**G4PenelopeCompton**)
  - Based on analytical calculations
- A “private” implementation has been around for a few years (*G4LECS by M. Kippen, New Astron. Rev. 48 (2004) 221–225*)
  - Beware: the code contains public data members!
- **Geant4 9.2-beta**: added also to the process based on the Livermore Library (**G4LowEnergyCompton**) and its polarized version (**G4LowEnergyPolarizedCompton**)
  - Same method as in EGS (Namito et al.), based on “Compton profiles”
  - Extension of data management capabilities

# Physics performance

Compton scattering of 40 keV photons on Si  
Energy distribution of photons  $89^\circ - 91^\circ$



# Computational performance

Test on an Intel Core2 Duo Processor E6420, 2.13 GHz, 4 GB RAM  
1M calls to **PostStepDoIt** function of Compton processes, 40 keV photons

Target	Livermore-based (s)	Penelope-based (s)	Speed factor
<b>C</b>	5.60	6.08	<b>8.6%</b>
<b>Si</b>	6.01	8.37	<b>39.3%</b>
<b>Cu</b>	6.17	10.78	<b>74.7%</b>
<b>W</b>	7.07	19.18	<b>271.3%</b>

*Weak dependency on photon energy in the range relevant to Doppler broadening*

Some thought about the toolkit strategy would be useful...

# From **cells** to **plasma**...

## Charge transfer

Relevant to astrophysics and plasma physics (e.g. fusion reactors)

New design technique introduced in Geant4:  
**policy-based class design**

*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

**Prototype development** to explore suitability of the design in other domains than microdosimetry

## Proton **charge transfer** processes for 12 materials

(He, water vapour, N<sub>2</sub>, CO, CO<sub>2</sub>, hydrocarbons)

**Cross sections**

ORNL/UGA Charge Transfer Database for Astrophysics  
+ other sources in literature

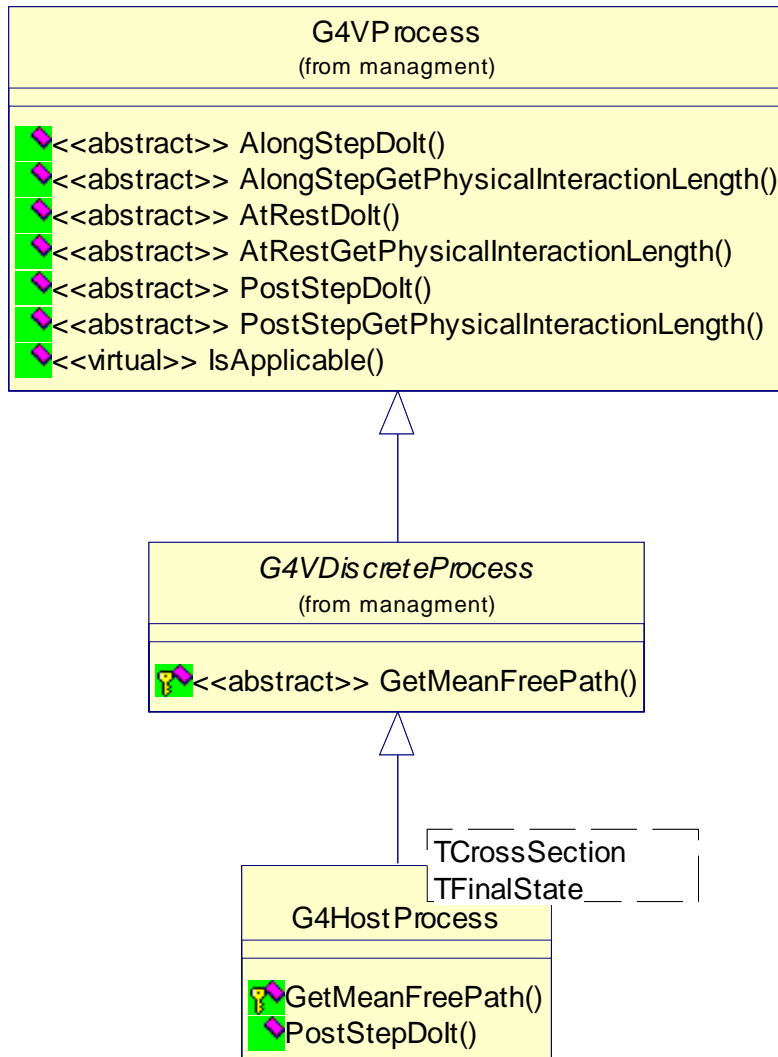
**Final state**

specific development for Geant4 implementation

**Development metrics**  
in **Easter egg**

**Design investment pays back!**

# Policy-based design of Geant4 processes



Handled transparently by Geant4 kernel

A **policy** defines a **class** or **class template interface**  
**Policy host classes** are **parameterised** classes

**Weak dependency** of the policy and the policy  
based class on the policy interface  
*Syntax-oriented rather than signature-oriented*

Advantage w.r.t. a conventional strategy pattern

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

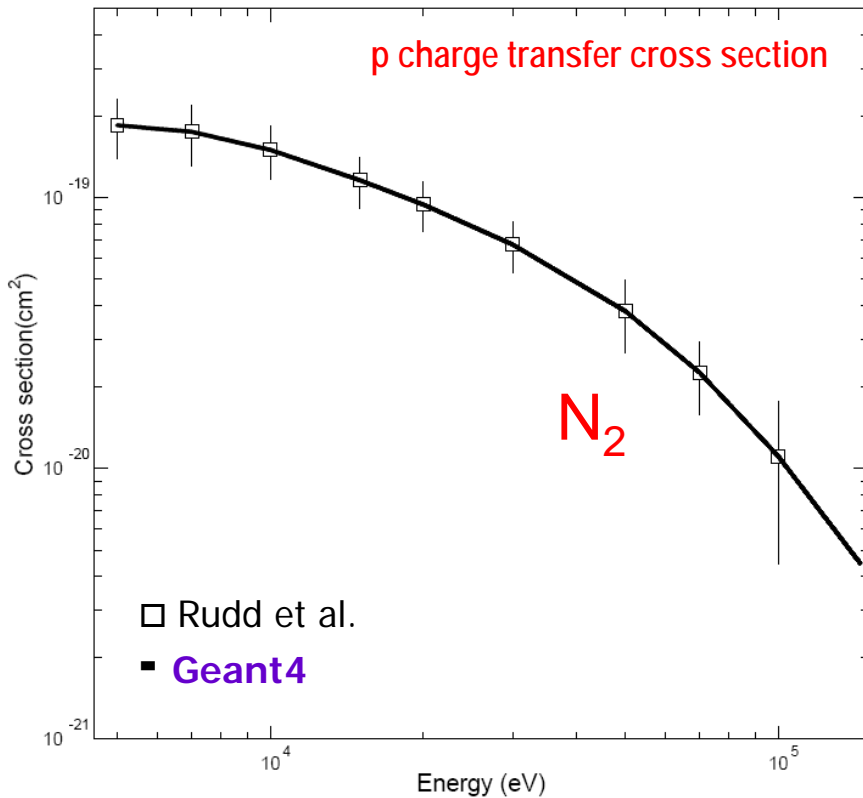
## Physics process class

Deprived of any intrinsic physics  
functionality

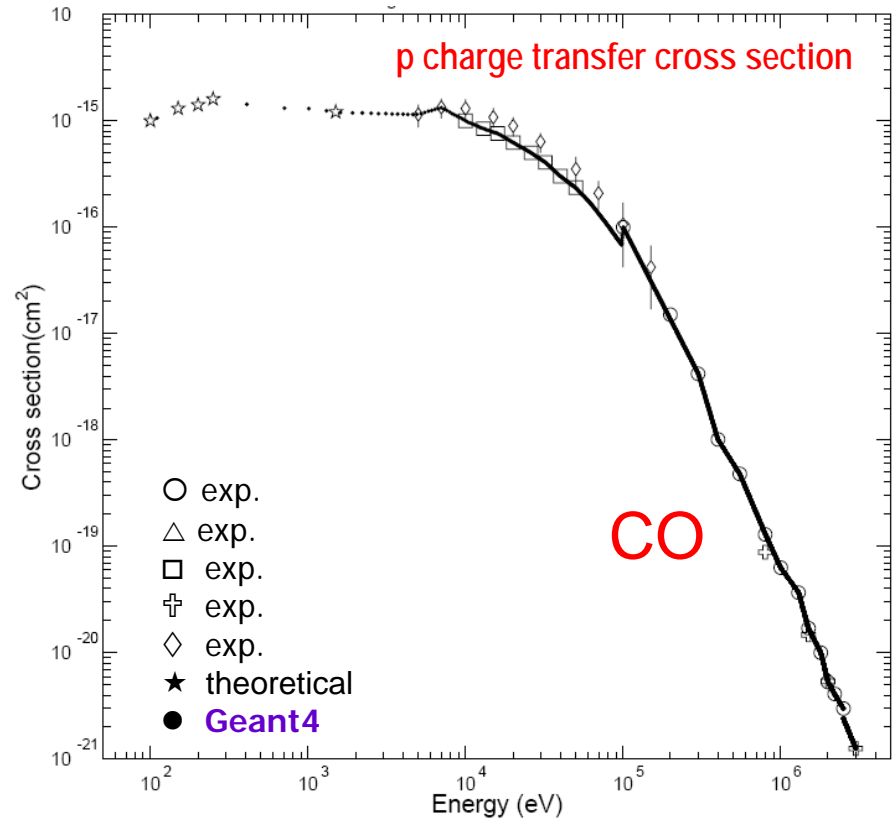
Configured by **template specialization**  
to acquire physics properties  
**Policy classes:** CrossSection, FinalState

# Examples of cross section models

## Analytical cross section model



## Data-driven cross section model



Transparent treatment of analytical  
and data-driven models

- M.E. Rudd et al., *Phys. Rev. A* 28, 3244-3257, 1983  
 L.H. Toburen et al., *Phys. Rev* 171, 114 - 122, 1968  
 S.L. Varghese et al., *Phys. Rev. A* 31, 2202-2209, 1985  
 M.B. Shah and H.B. Gilbody, *J. Phys. B* 23, 1491-1499, 1990  
 R.S. Gao et al., *Phys. Rev. A* 41, 5929-5933, 1990  
 M. Kimura et al., *Phys. Rev. A* 61, 032708, 2000

# Outlook

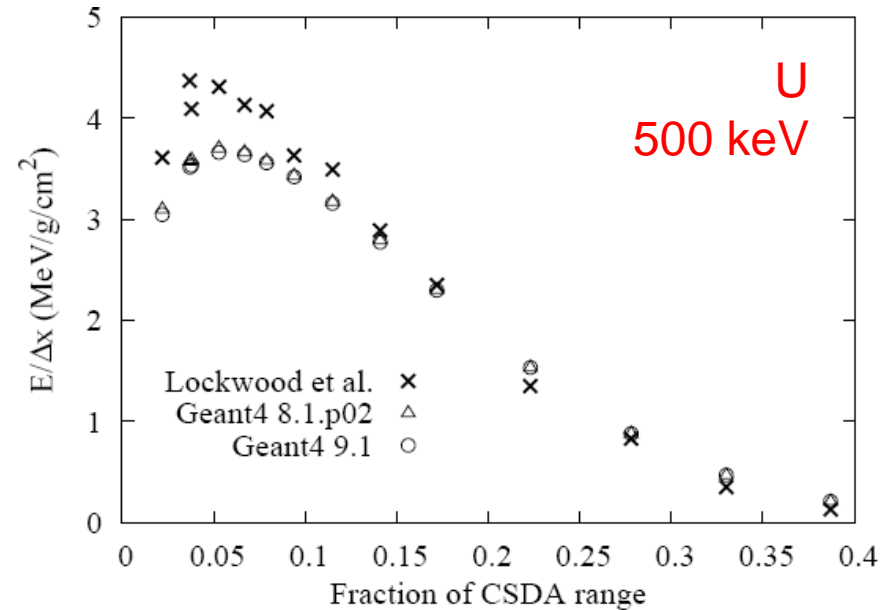
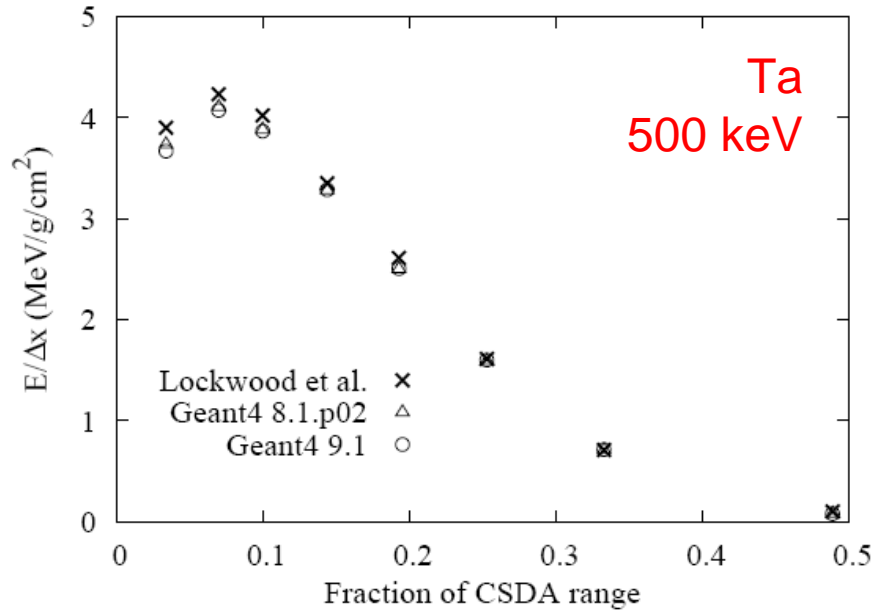
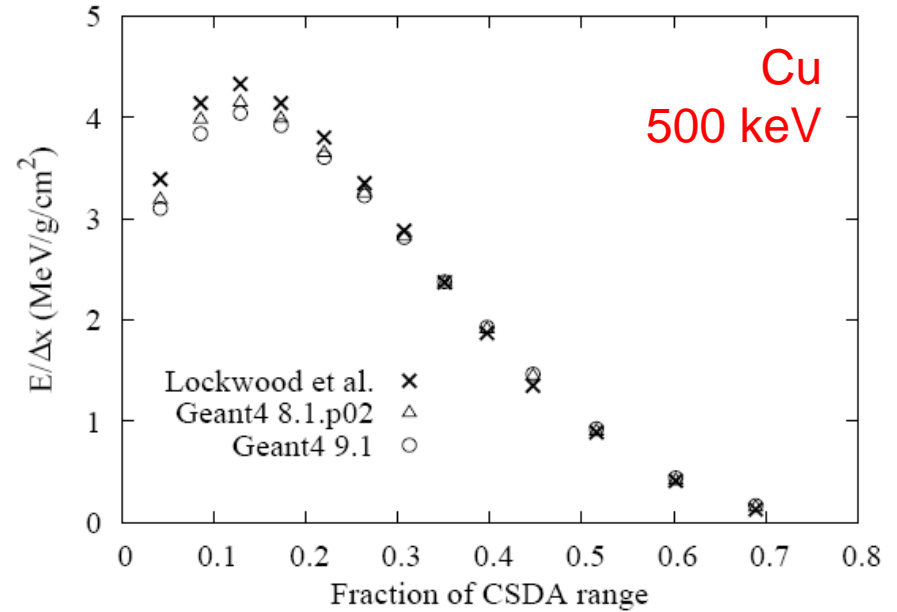
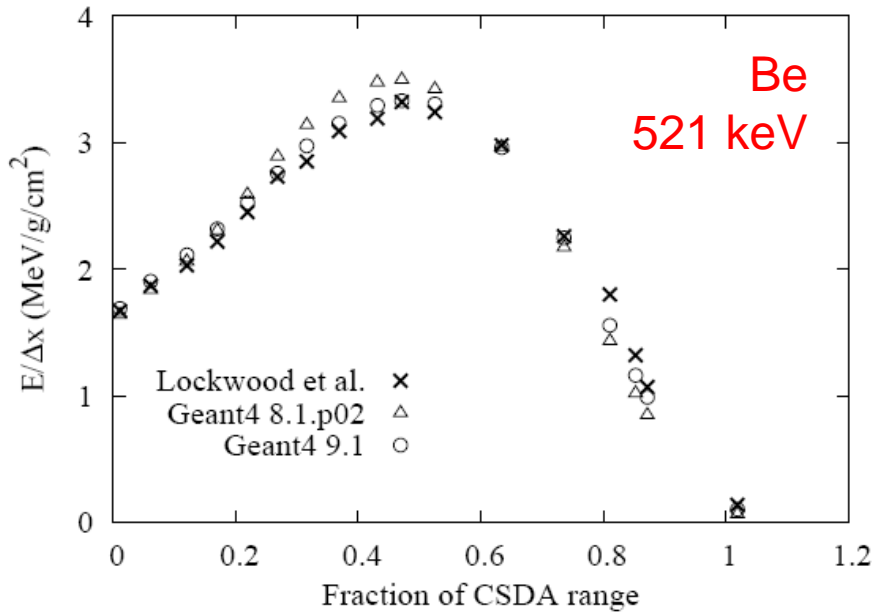
- Feedback from the experimental community
  - Interest?
  - Priorities?
- Process design and implementation is trivial
  - Provided cross sections are available
- How to deal with ion charge state proliferation efficiently?
- Is Geant4 physics sensitive to ion charge?
- What about other ion interactions?
- Issue to be addressed in new R&D project recently launched at INFN
  - “mutant” entities in particle transport



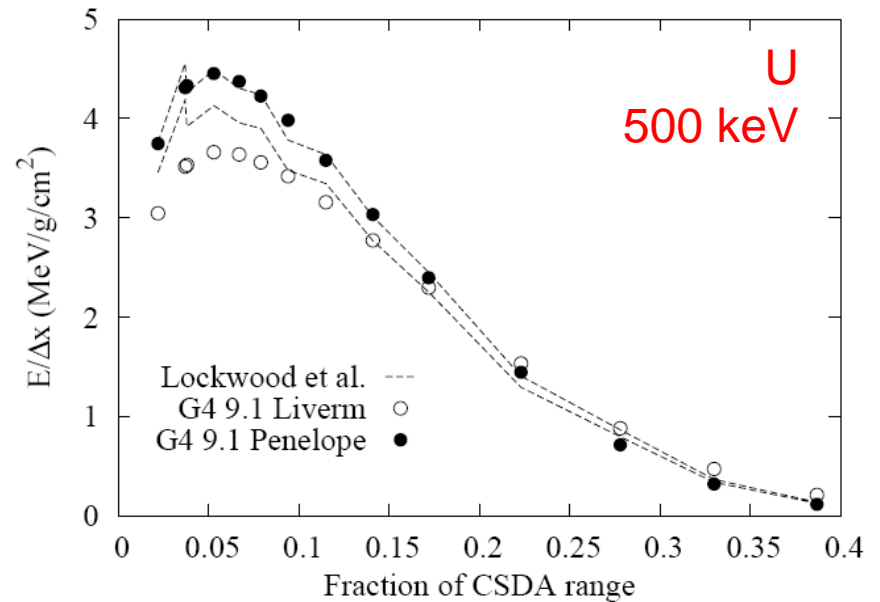
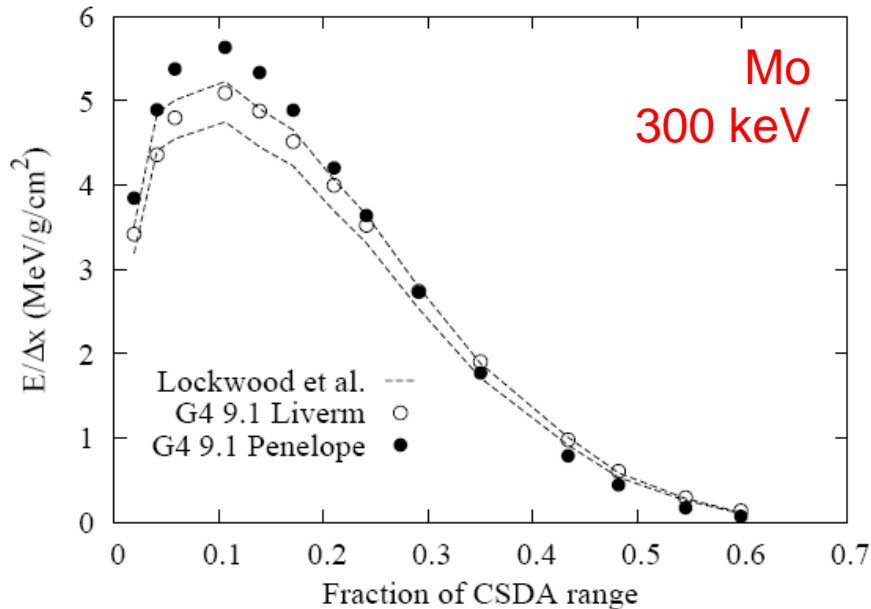
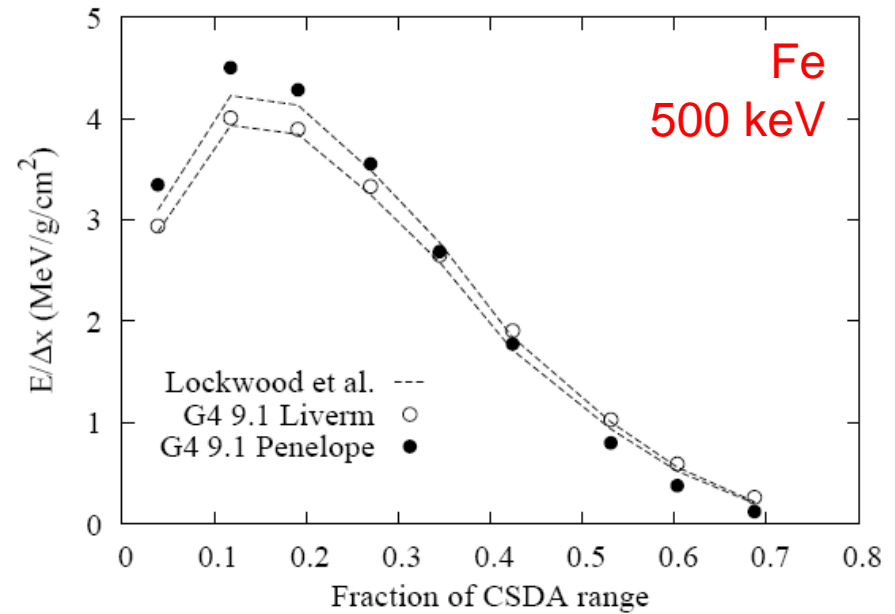
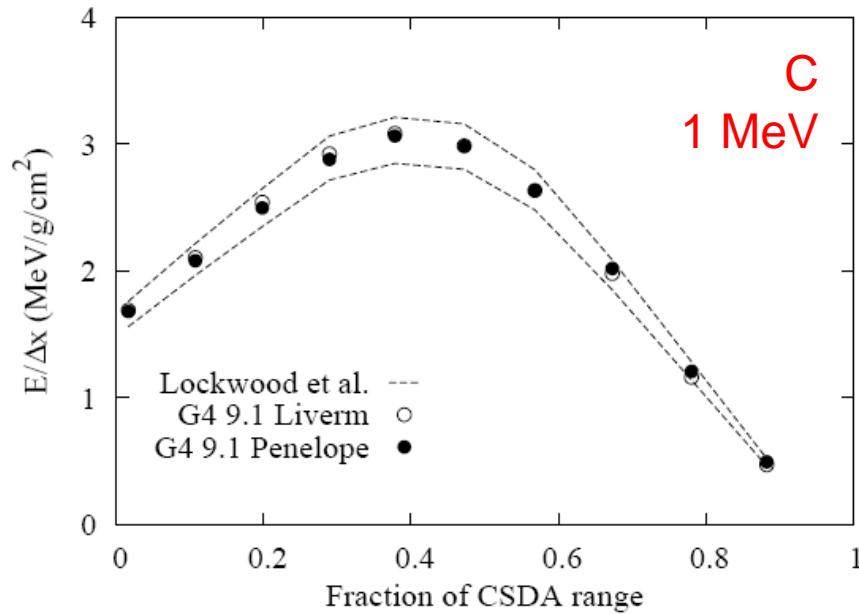
# Validation of low energy electrons energy deposit

- Experimental data from G. J. Lockwood et al., “*Calorimetric Measurement of Electron Energy Deposition in Extended Media - Theory vs Experiment*”, SAND79-0414
  - 50 keV – 1 MeV electrons on **Be, C, Fe, Cu, Al, Mo, Ta, U**
  - 90°, 60°, 30° beam incidence angle
  - Errors: 1.2 – 2.2 % (depending on material)
- **Livermore Library-based and Penelope-like processes**
  - Penelope models as implemented in Geant4 (Geant4-native multiple scattering)
- **Geant4 9.1 and 8.1**
  - Check evolution of **multiple scattering** implementation
  - *other processes unchanged between 8.1 and 9.1 versions*
- **Rigorous statistical analysis**
  - Quantitative evaluation of the two models implemented in Geant4
  - Objective guidance for users’ **PhysicsLists**

# Some results, Geant4 8.1p02 vs. 9.1



# Library-based vs. Penelope-like processes



# $\chi^2$ test results, 90°

Consistent results from unbinned goodness-of-fit tests  
(Kolmogorov-Smirnov, Anderson-Darling, Cramer-von Mises, Watson, Kuiper)

Material	Energy (MeV)	p-value library-based Geant4 8.1p02	p-value library-based Geant4 9.1	p-value Penelope-like Geant4 9.1
Beryllium	0.058	0.021	0.025	0.002
	0.109	< 0.001	1	< 0.001
	0.314	< 0.001	0.019	< 0.001
	0.521	< 0.001	0.261	0.330
	1.033	< 0.001	< 0.001	0.171
Carbon	1	0.220	0.885	0.996
Aluminium	0.314	< 0.001	0.376	0.200
	0.521	0.002	0.133	0.497
	1.033	< 0.001	0.015	0.001
Iron	0.3	0.039	0.534	< 0.001
	0.5	0.520	0.092	< 0.001
	1	0.017	0.001	< 0.001
Copper	0.3	0.032	< 0.001	< 0.001
	0.5	0.025	< 0.001	< 0.001
Molybdenum	0.1	< 0.001	< 0.001	< 0.001
	0.3	0.028	0.027	< 0.001
	0.5	0.096	0.015	< 0.001
	1	< 0.001	< 0.001	< 0.001
Tantalum	0.3	0.048	0.086	< 0.001
	0.5	0.155	0.035	< 0.001
	1	0.079	0.031	< 0.001
Uranium	0.3	< 0.001	< 0.001	< 0.001
	0.5	< 0.001	< 0.001	< 0.001
	1	< 0.001	< 0.001	< 0.001

## Null hypothesis

Compatibility of experimental and simulated energy deposit profiles

## Confidence level

for the rejection of the null hypothesis: 99%

## Analysis

By single configuration  
By category

# Geant4 8.1 vs. 9.1 (multiple scattering)

Geant4 **8.1p02** and **9.1** difference evaluated by means of **contingency tables**

**Improved accuracy in light materials, same for heavy materials, controversial for Fe-Cu**

## All data 90°

$\chi^2$ test outcome	Geant4 8.1p02	Geant4 9.1
Pass	12	15
Fail	12	9
p-value Fisher	0.561	
p-value Pearson	0.383	
$\chi^2$	0.383	
p-value Yates $\chi^2$	0.561	

## Be - C - Al

$\chi^2$ test outcome	Geant4 8.1p02	Geant4 9.1
Pass	2	8
Fail	7	1
p-value Fisher	0.015	

## Fe - Cu

$\chi^2$ test outcome	Geant4 8.1p02	Geant4 9.1
Pass	5	2
Fail	0	3
p-value Fisher	0.167	

## Mo - Ta

$\chi^2$ test outcome	Geant4 8.1p02	Geant4 9.1
Pass	5	5
Fail	2	2
p-value Fisher	1	

*No energy dependent differences observed*

# Library-based vs. Penelope-like processes

Livermore Library-based and Penelope-like difference evaluated through **contingency tables**

Complementary to comparison against NIST Physical Reference Data

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, 2005

## All data, 90°

$\chi^2$ test outcome	Library based	Penelope like
<b>Pass</b>	15	5
<b>Fail</b>	9	19
p-value Fisher	<b>0.008</b>	
p-value Pearson $\chi^2$	<b>0.003</b>	
p-value Yates $\chi^2$	<b>0.008</b>	

## $E \leq 314$ keV

$\chi^2$ test outcome	Library based	Penelope like
<b>Pass</b>	5	1
<b>Fail</b>	1	5
p-value Fisher	<b>0.080</b>	

## $314 < E \leq 521$ keV

$\chi^2$ test outcome	Library based	Penelope like
<b>Pass</b>	5	2
<b>Fail</b>	1	4
p-value Fisher	0.242	

## $E > 521$ keV

$\chi^2$ test outcome	Library based	Penelope like
<b>Pass</b>	3	2
<b>Fail</b>	3	4
p-value Fisher	0.999	

*No material dependent differences observed*

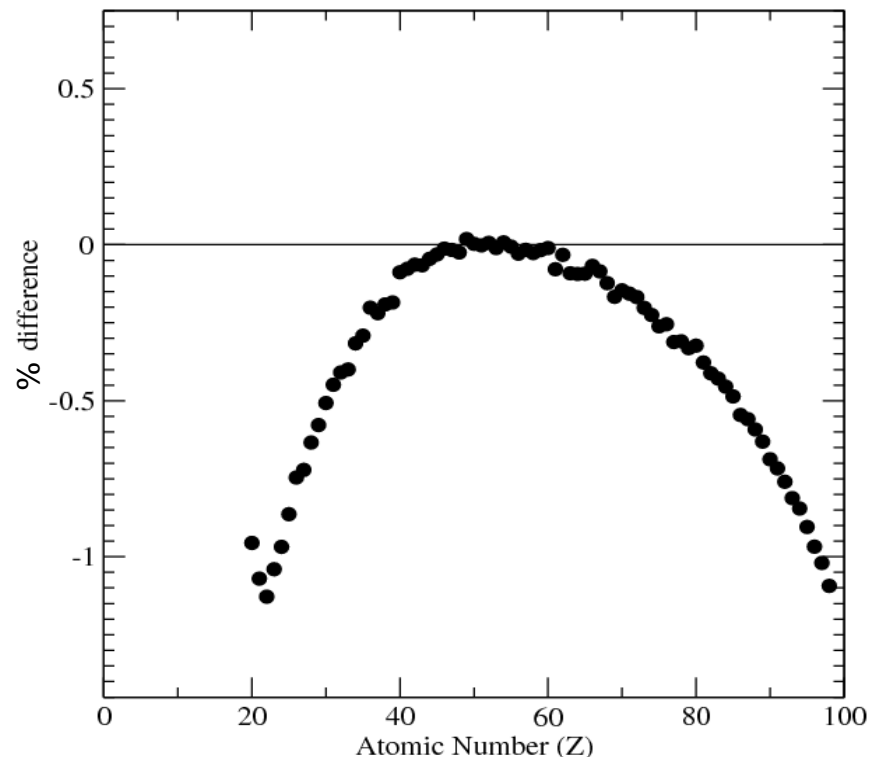
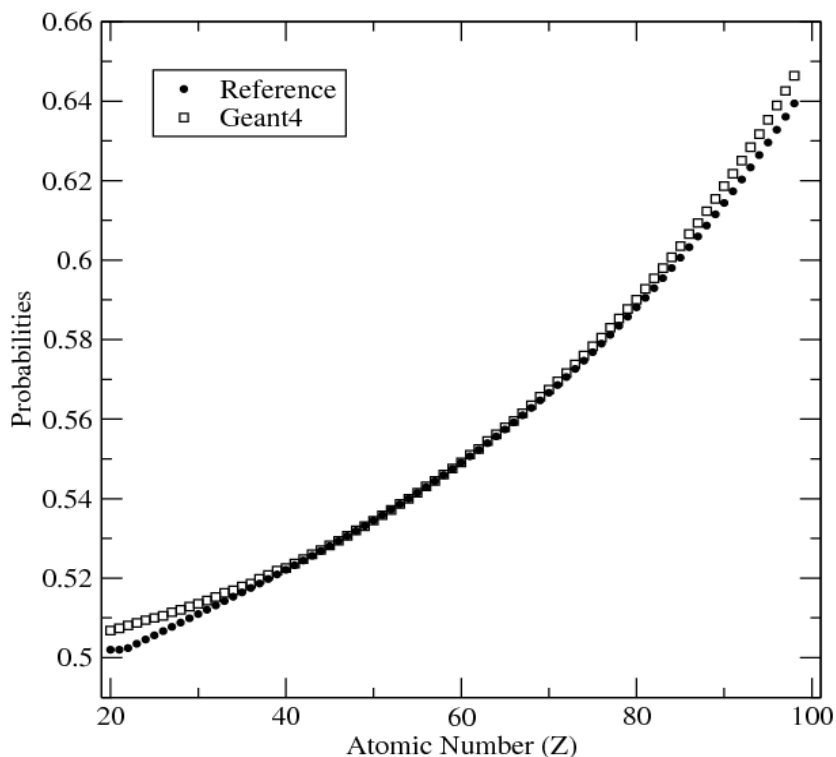
## Geant4 Atomic Relaxation

Susanna Guatelli, Alfonso Mantero, Barbara Mascialino, Petteri Nieminen, and Maria Grazia Pia

Validation of Geant4 Atomic Relaxation Against the  
NIST Physical Reference Data

S. Guatelli, A. Mantero, B. Mascialino, M. G. Pia, and V. Zampicelli

## Validation of Fluorescence Transition Probabilities

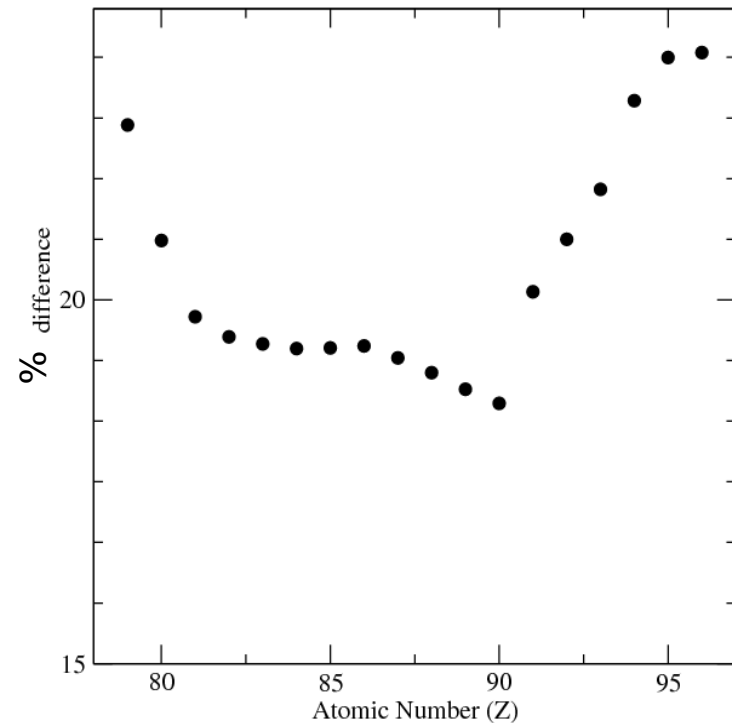
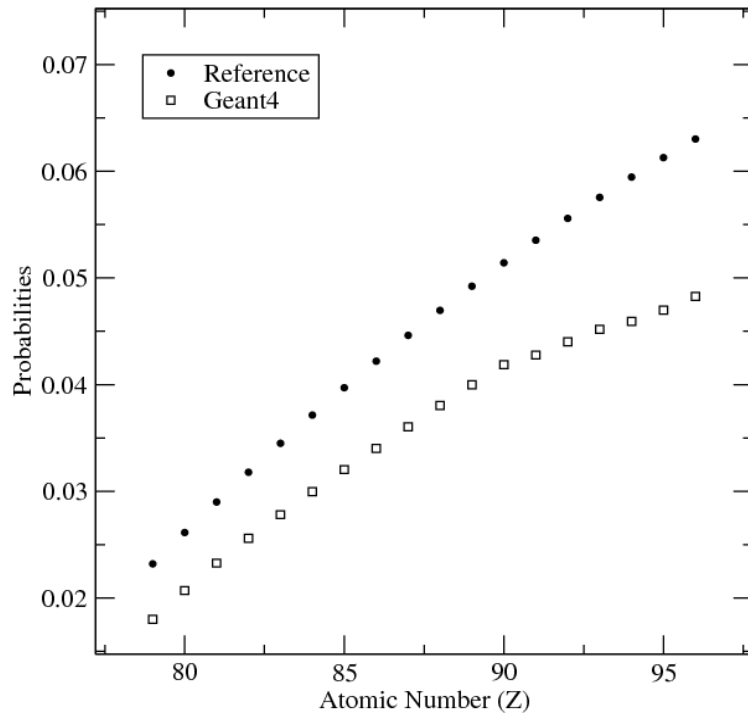
KL<sub>2</sub> transitions

Experimental reference:

W.T. Elam, B.D. Ravel, J.R. Sieber, *A new atomic database for X-ray spectroscopic calculations*, Radiat. Phys. Chem. 63 (2002) 121–128

# Bad but harmless...

$L_3 O_{4,5}$  transitions

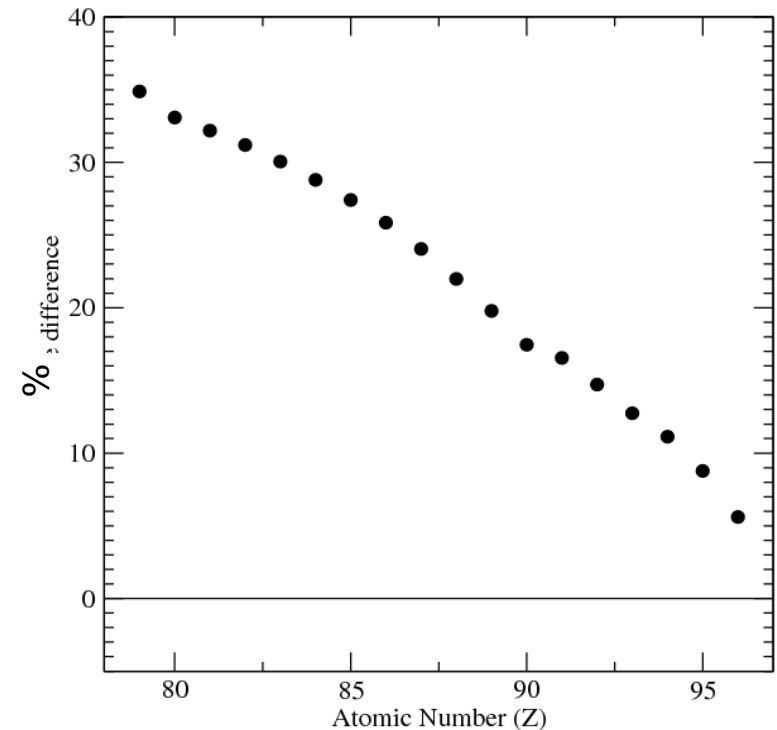
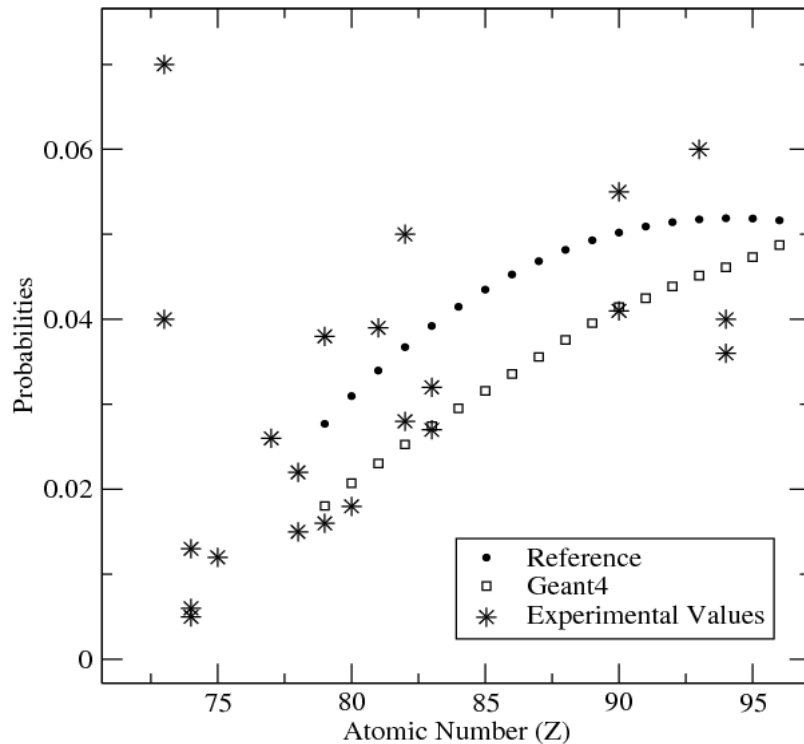


25% absolute error  $\Rightarrow$  0.04% error in an experimental use case



# Hard to say...

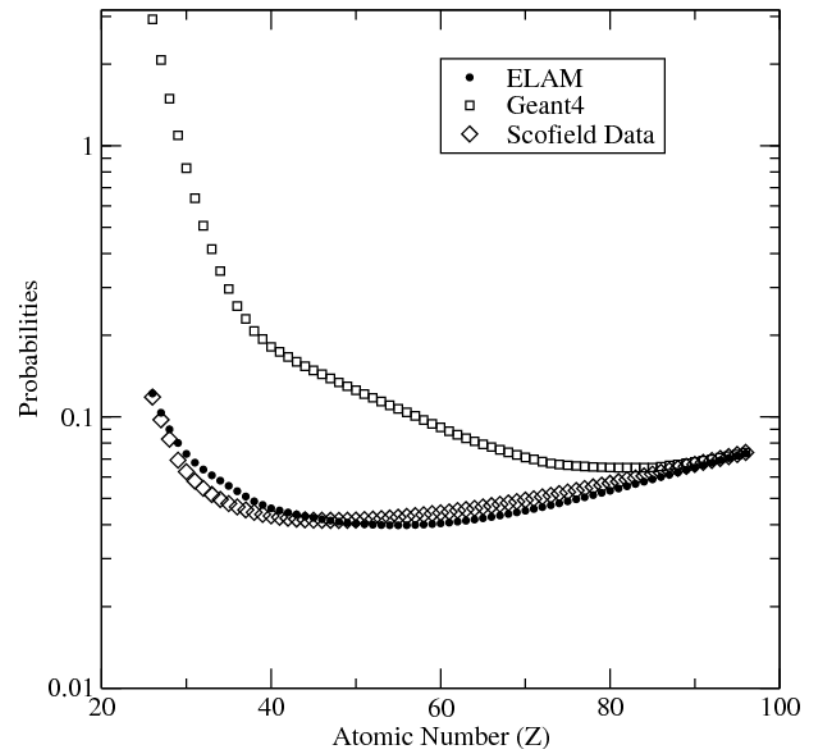
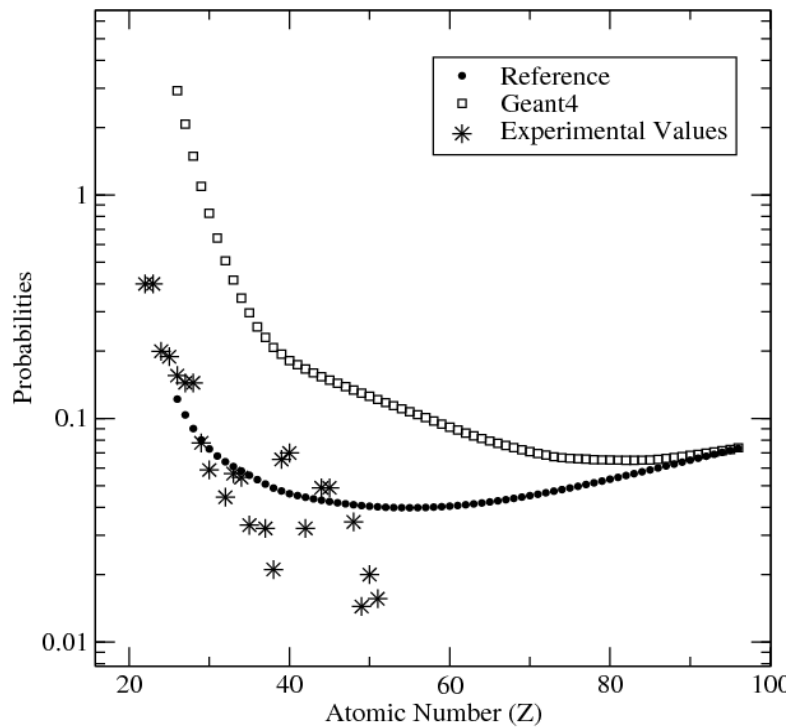
## $L_2 O_4$ transitions



Controversial experimental data

# Hidden for 17 years...

## $L_3 M_1$ transitions



**The error is in EADL!**

# Conclusion and outlook

- Rich physics coverage, continuously expanding
- Ongoing validation... sometimes with surprises
- Geant4 10th birthday, RD44 14th birthday

## New experimental domains

Nanotechnologies, new power plants, radiobiology etc.

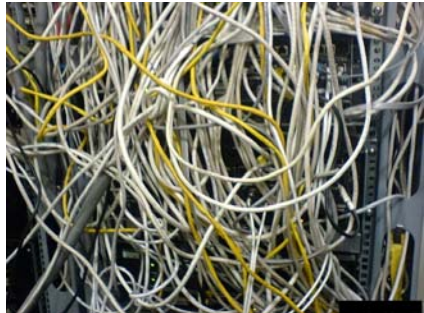
## New software technologies

Generic/Generative programming, Aspect Oriented programming etc.

## Lessons learned

In developing and using Geant4

## R&D project to revisit Geant4 design and core capabilities



1<sup>st</sup> stage, then...

**Condensed - discrete transport schemes**

**Monte Carlo - deterministic transport schemes**