



## PIXE Simulation

### Models, methods and technologies

Maria Grazia Pia  
*INFN Genova, Italy*  
[maria.grazia.pia@cern.ch](mailto:maria.grazia.pia@cern.ch)



M. Batič<sup>1,2</sup>, P. Saracco<sup>1</sup>, G. Weidenspointner<sup>3</sup>

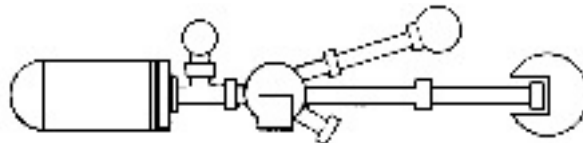
<sup>1</sup>*INFN Sezione di Genova, Italy*

<sup>2</sup>*Jozef Stefan Institute, Ljubljana, Slovenia*

<sup>3</sup>*Max-Planck-Institut für extraterrestrische Physik and Halbleiterlabor, Germany*

**CAARI 2012**

Maria Grazia Pia, *INFN Genova*



Fort Worth, Texas, USA  
5-10 August 2012

S. Agostinelli et al.

## **Geant4: a simulation toolkit**

*NIM A*, vol. 506, no. 3, pp. 250-303, 2003

# Geant 4

**3137 citations**

Most cited CERN publication in Web of Science<sup>SM</sup>  
(excluding *Rev. Part. Properties*)

## **Nuclear Science & Technology Instruments & Instrumentation**

J. P. Biersack and L. G. Haggmark,

### **A Monte-Carlo computer-program for the transport of energetic ions in amorphous targets**

*NIM*, vol.174, no. 1-2, pp. 257-269, 1980

**3627 citations**

L. R. Doolittle,

### **Algorithms for the rapid simulation of Rutherford backscattering spectra**

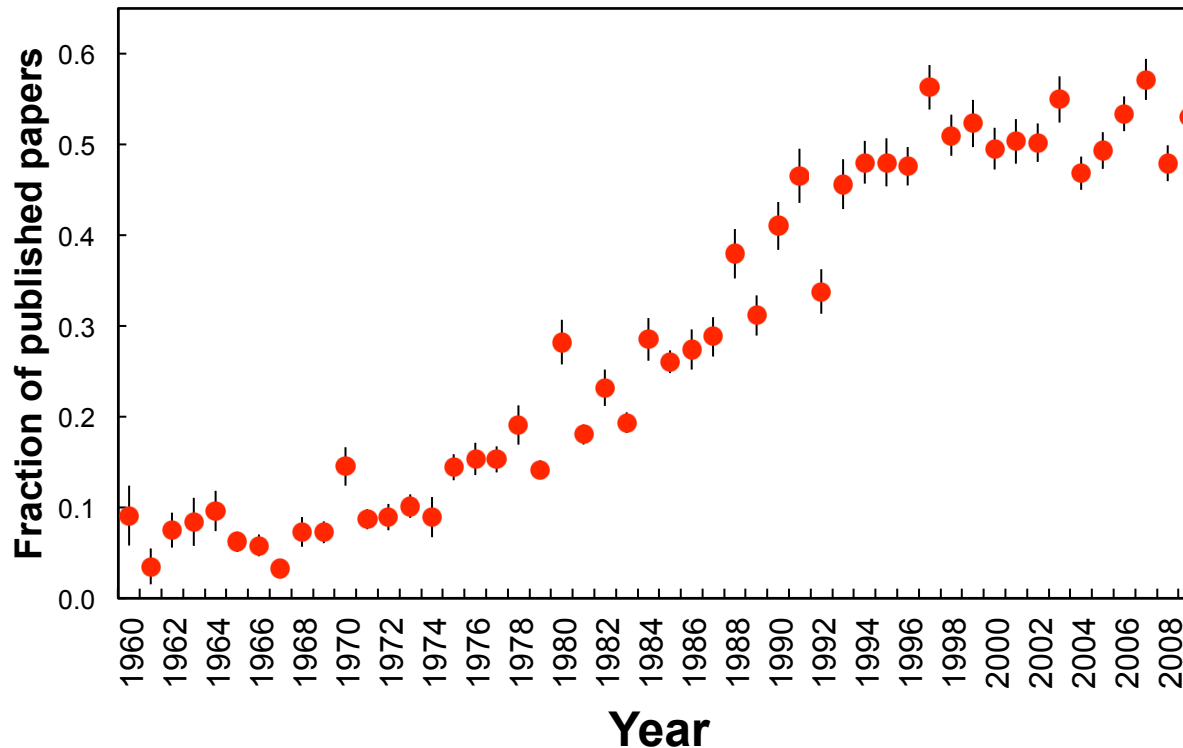
*NIM B*, vol. 9, no. 3, pp. 344-351, 1985

**2071 citations**

Source: Thomson-Reuters, Web of Science<sup>SM</sup> (7 August 2012)

# Monte Carlo simulation in literature

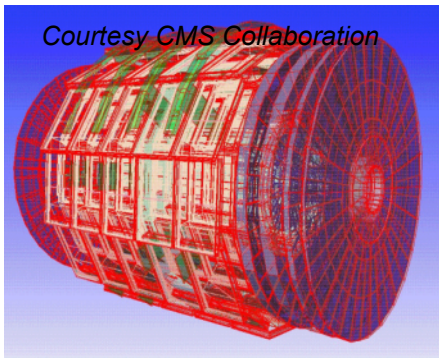
**Fraction of IEEE TNS papers mentioning Monte Carlo or simulation**



Same trend  
in NIM

M. G. Pia, T. Basaglia, Z.W. Bell, P.V. Dressendorfer

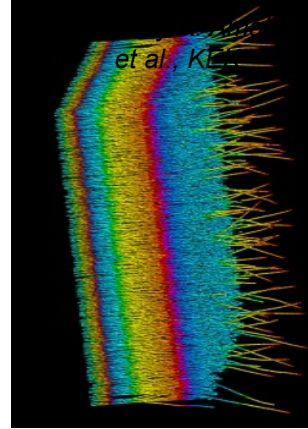
The butterfly effect: correlations between modeling in nuclear-particle physics and socioeconomic factors



# Geant 4

## Object oriented toolkit

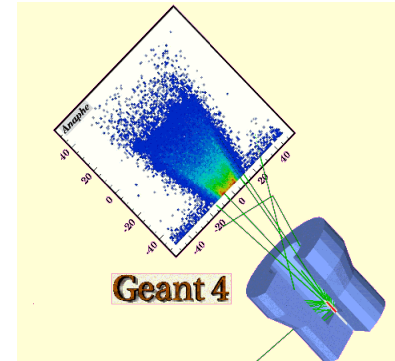
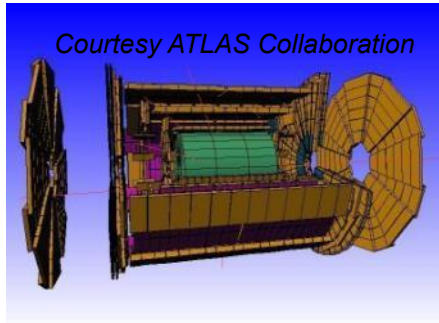
for the simulation of particle interactions with matter



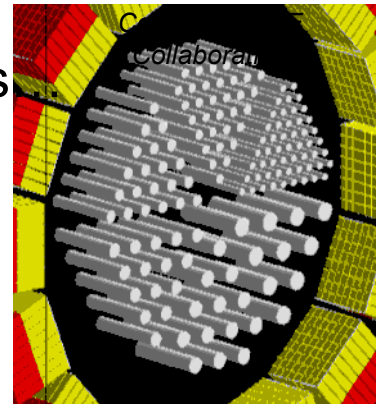
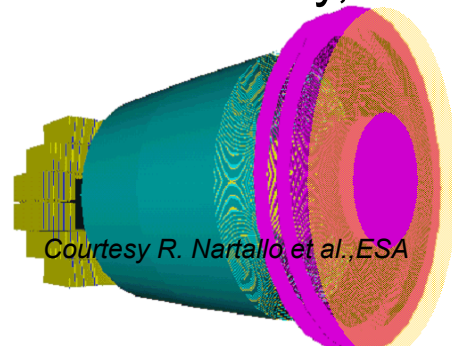
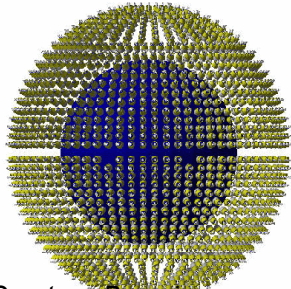
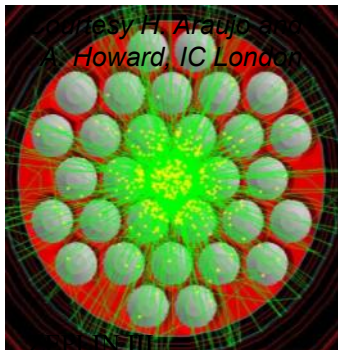
## Born from the requirements of large scale HEP experiments

Widely used in:

- Space science and astrophysics
- Medical physics, nuclear medicine
- Radiation protection
- Accelerator physics
- Pest control, food irradiation
- Humanitarian projects, security
- etc.
- Technology transfer to industry, hospitals



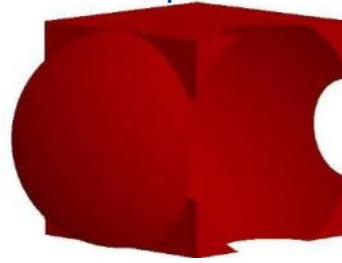
IST and INFN  
Genova



Maria Grazia Pia, INFN Courtesy Borexino

# Geometry

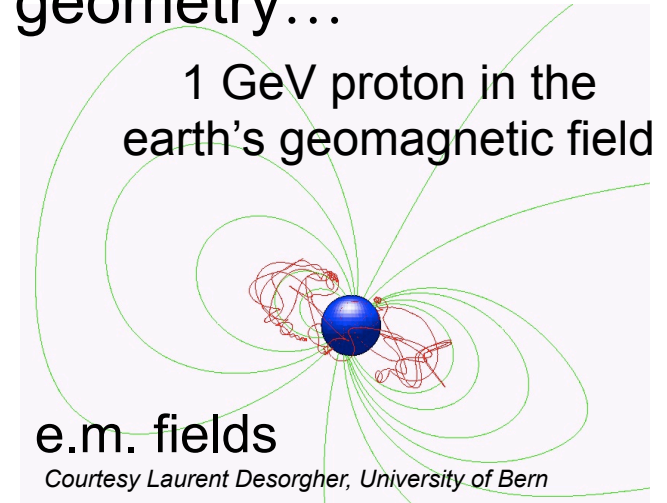
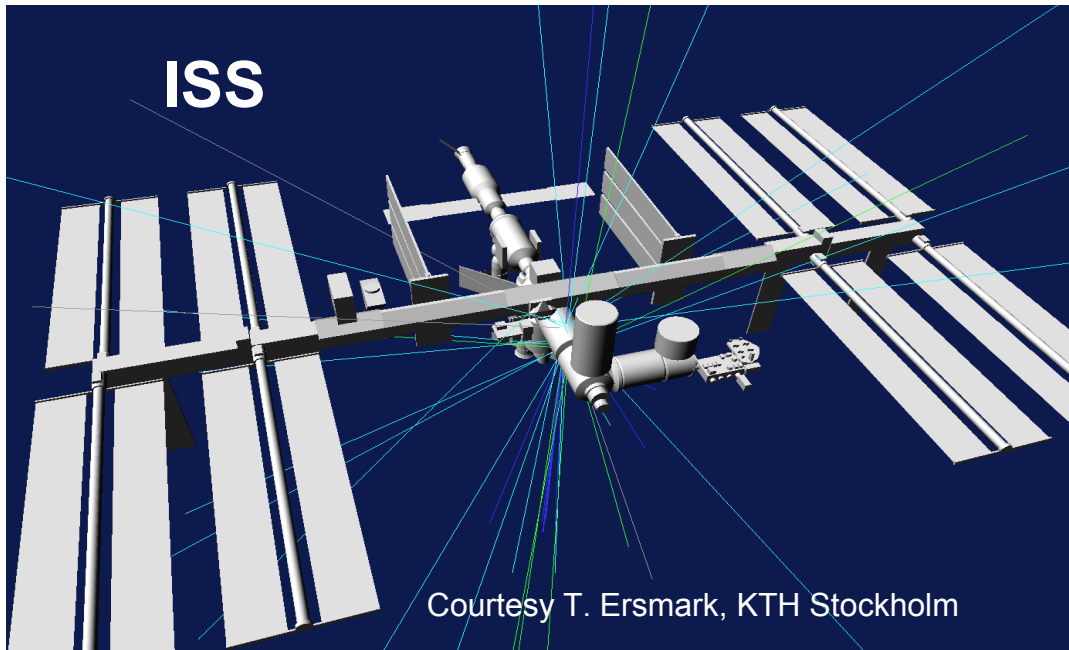
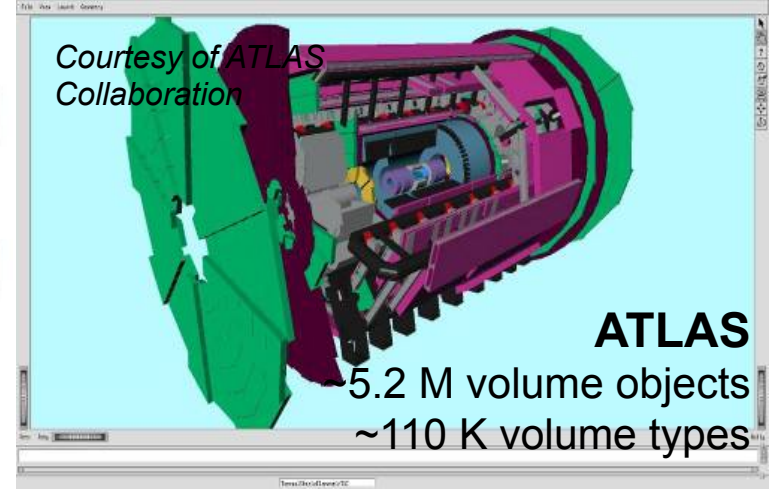
Boolean operations



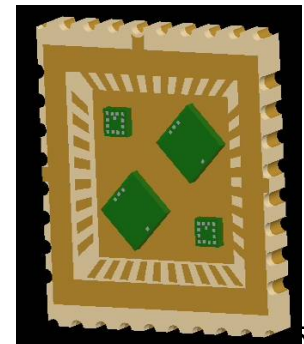
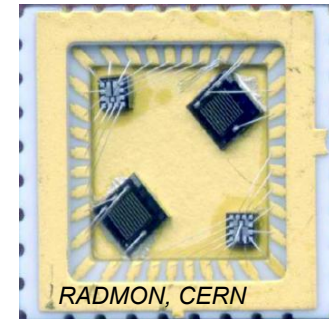
## ● Role

- detailed detector description
- efficient navigation across volumes

## ● One can do fancy things with Geant4 geometry...



Maria Grazia Pia, *INFN Genova*



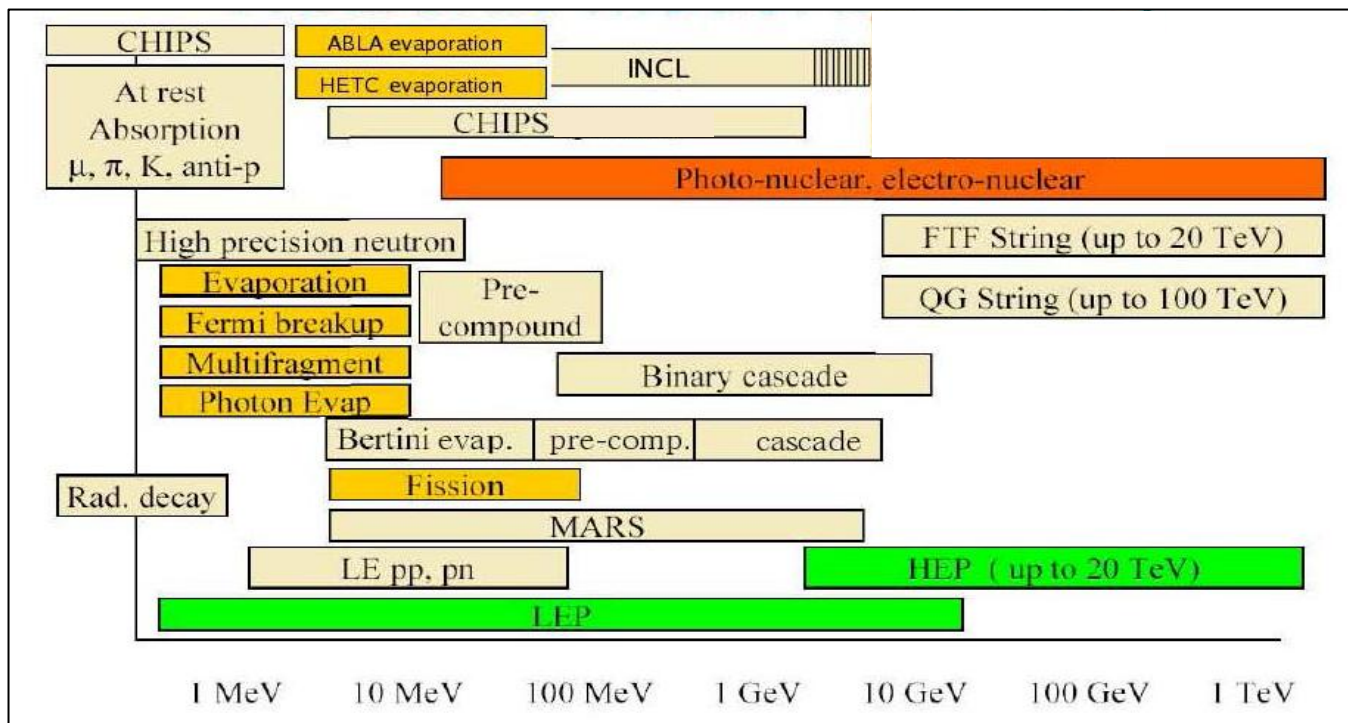
# Physics

## Electromagnetic

- electrons and positrons
- photons (including optical photons)
- muons
- charged hadrons
- ions

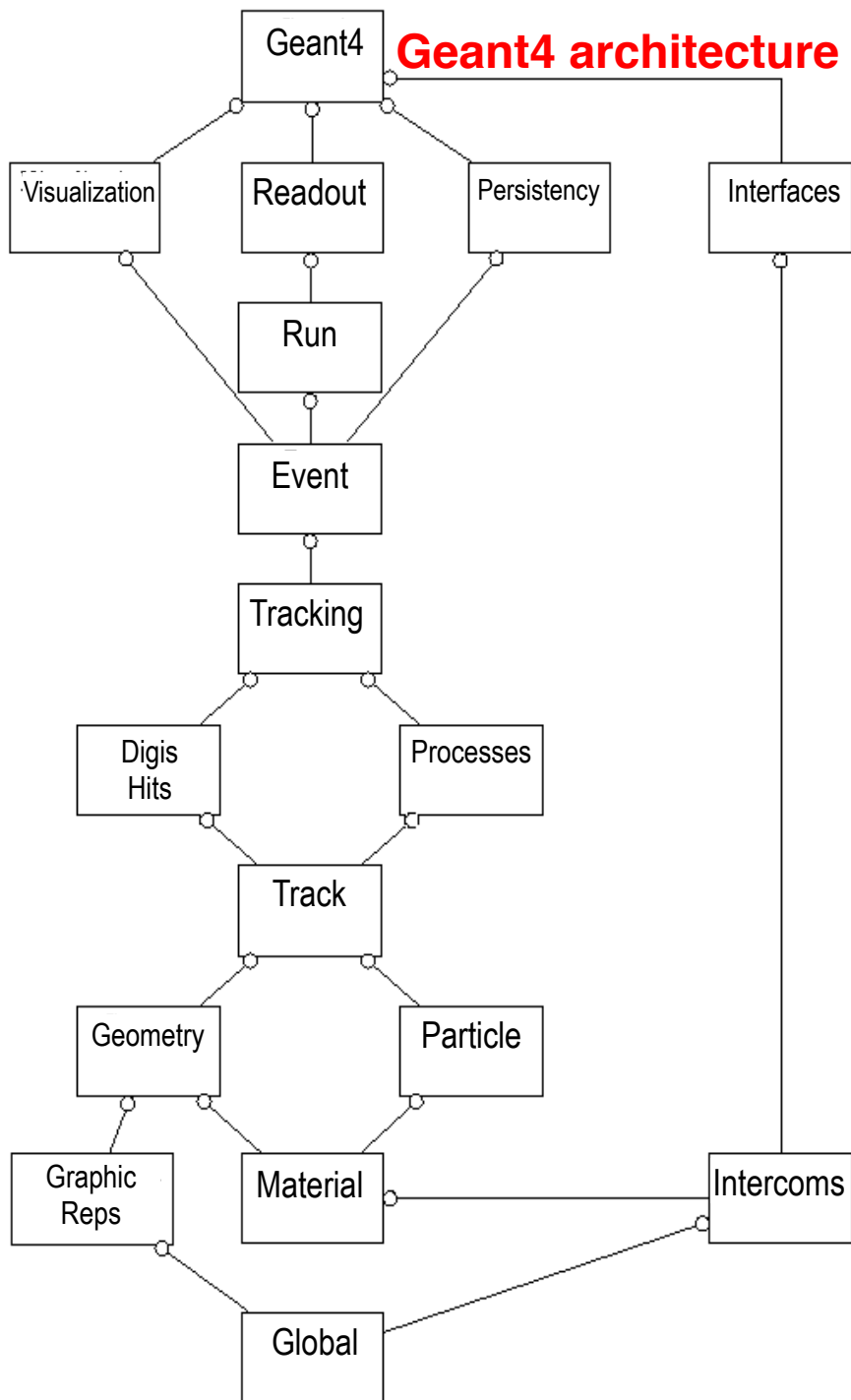
Multiple scattering  
 Bremsstrahlung  
 Ionisation  
 Annihilation  
 Photoelectric effect  
 Compton scattering  
 Rayleigh scattering  
 $\gamma$  conversion

Synchrotron radiation  
 Transition radiation  
 Cherenkov  
 Refraction  
 Reflection  
 Absorption  
 Scintillation  
 Fluorescence  
 Auger emission



## Hadronic

- Theory-driven
- Parameterized
- Data-driven



# Geant 4

Open source code

Freely available

Source code, libraries, data files, documentation

<http://cern.ch/geant4>

Developed and managed by an international team of scientists

Open to contributions from the scientific community

# PIXE in Geant4 (and other codes)

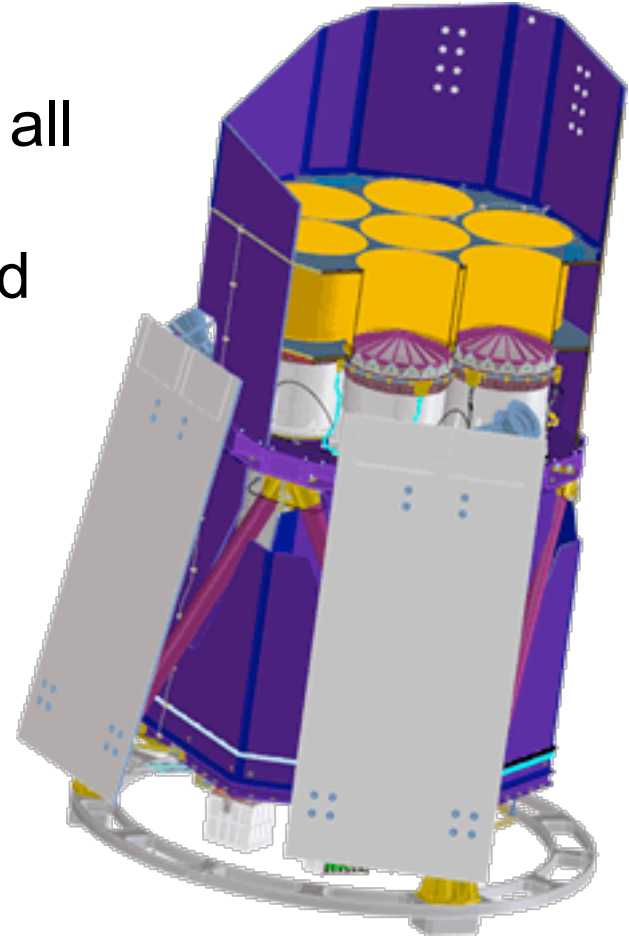
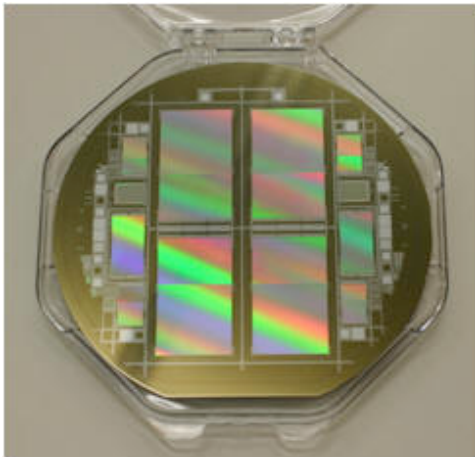
- **Specialized codes for PIXE analysis (and simulation)**
  - GeoPIXE, GUPIX, PIXAN, PixeKLM, Sapix, WinAxil, Wits-HEX etc.
  - DATTPIXE, DT2, LibCPIXE, VIBA-Lab1/2 etc.
  - Concerned with experimental observables relevant to material analysis
- **Impact ionisation by electrons**
  - EGS\*, Geant4, Penelope
  - Cross sections available for all shells
- Geant4 R&D with PIXE started in 2001
- Major step forward in 2008
- Further refinements in progress
- Open to evolution: OO technology + physics



# eROSITA

extended **R**oentgen **S**urvey with  
an **I**maging **T**elescope **A**rray

Systematic detection and analysis of all  
obscured accreting Black Holes in  
nearby galaxies and of ten thousand  
galaxy clusters

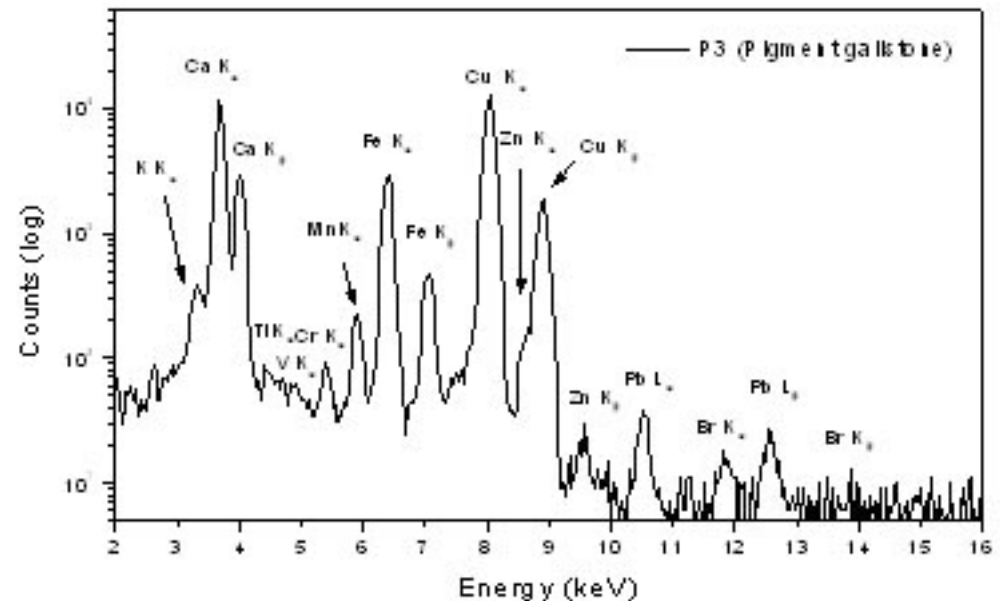
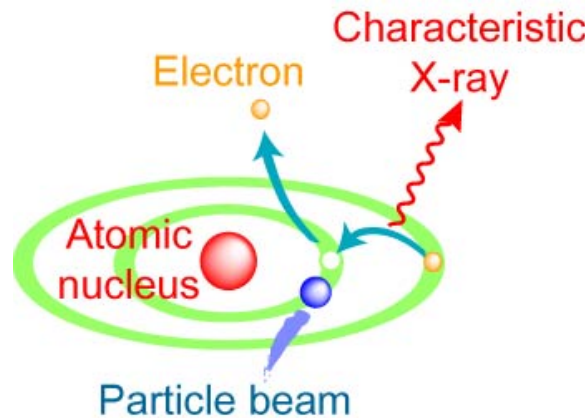


On-board the Russian "Spectrum-Roentgen-Gamma" (SRG) satellite  
to be launched from Baikonur in 2013 and placed in an L2 orbit

# PIXE

## Particle Induced X-ray Emission

Particle = proton, ion (electron)



The physics of PIXE is simple

The simulation of PIXE is **NOT** simple

interplay of **continuous** and **discrete transport methods**

# PIXE simulation recipe

## Ingredients

Specific to PIXE

- Proton (ion) **ionisation cross sections** for individual shells
- Radiative and non-radiative **transition probabilities**
- Atomic **binding energies** (X-ray energies)

## Instructions

- **Create a vacancy** in the shell occupancy due to ionisation
- **De-excite** the atom through fluorescence and Auger emission

## A touch of spice

**Infrared divergence** of the cross section for  $\delta$ -ray emission

Monte Carlo codes neutralize the spice by introducing “**cuts**”  
(i.e. a threshold for  $\delta$ -ray production)

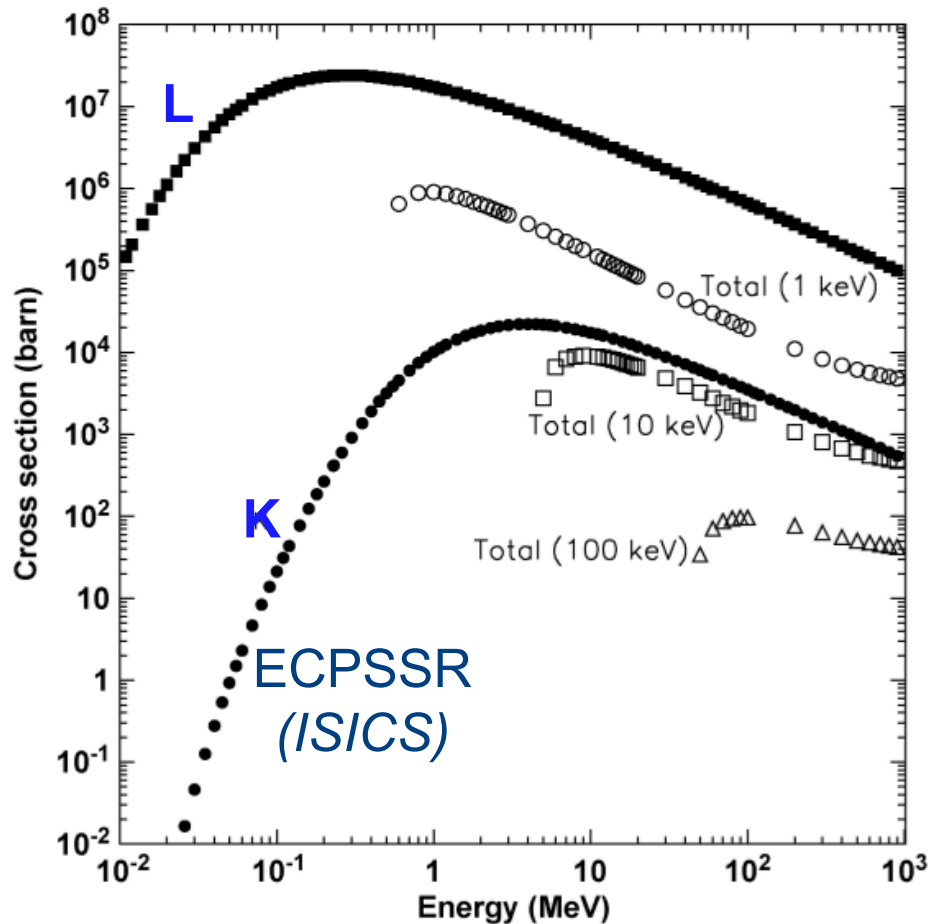
Below the threshold: ionisation treated as *continuous energy loss*  
Above the threshold: *emission of an electron*

PIXE is and intrinsically **discrete** process, which is intimately associated with a **continuous-discrete** one

## Note

One of the ingredients (ionisation cross sections) is available in limited quantity (for a few **inner shells only**)

# Condensed-discrete ionisation



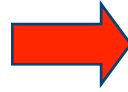
Si ionisation by protons

Depending on the  $\delta$ -ray production cut, the “total” cross section may be **smaller** than the **K shell** ionisation cross section

Can we deal with PIXE consistently?

- What can we do with existing instruments?
- Longer term R&D on transport methods

Determination of a  
vacancy



Relative probability of  
ionising a shell w.r.t. the  
other shells

But we **do not know** the total ionisation cross section  
*(without introducing a dependency on cuts)*

We can calculate ionisation cross sections only for K, L, M shells

OK for light elements

OK for relative estimates

Overestimate inner shell vacancies for heavier elements

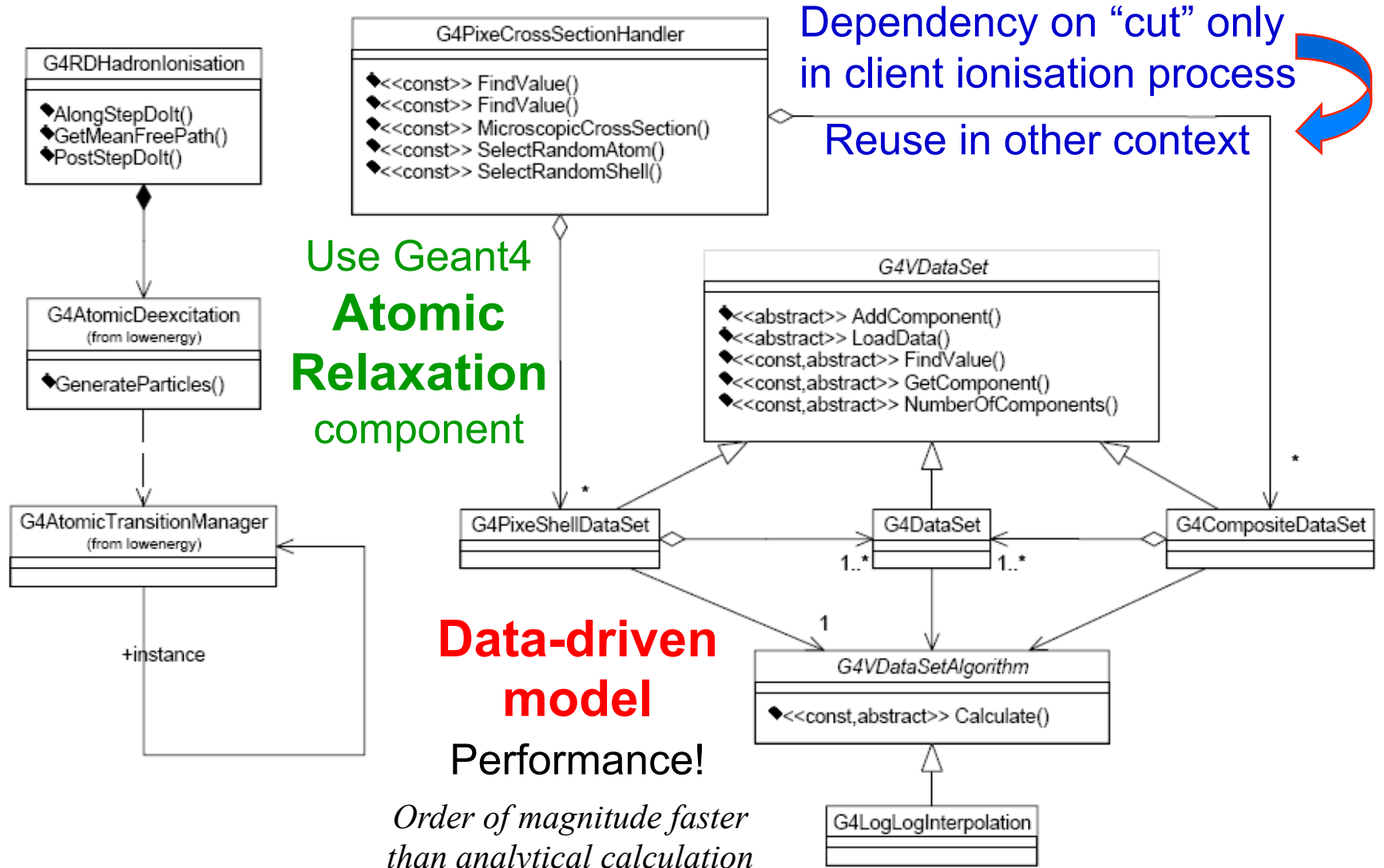
*In principle, the issue would be solved if we could  
calculate ionisation cross sections for all shells*

## PIXE Simulation With Geant4

Maria Grazia Pia, Georg Weidenspointner, Mauro Augelli, Lina Quintieri, Paolo Saracco, Manju Sudhakar, and  
Andreas Zoglauer

# Domain decomposition

No dependence of PIXE component on  $\delta$ -ray production threshold



# Ionisation cross sections

## Proton, K shell

- PWBA
- ECPSSR
- ECPSSR Hartree-Slater
- ECPSSR United Atom
- ECPSSR relativistic
- Paul & Sacher
- Kahoul et al.

## Proton, L shell

- PWBA
- ECPSSR
- ECPSSR United Atom
- Miyagawa et al.
- Orlic et al.
- Sow et al.

## Proton, M shell

- PWBA
- ECPSSR
- ECPSSR United Atom

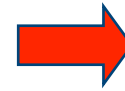
## $\alpha$ , K shell

- PWBA
- ECPSSR
- ECPSSR Hartree-Slater
- ECPSSR United Atom
- Paul & Bolik

## $\alpha$ , L and M shell

- PWBA
- ECPSSR
- ECPSSR United Atom

■ Theoretical  
■ Empirical



Released as  
**PIXE 2010**  
data library

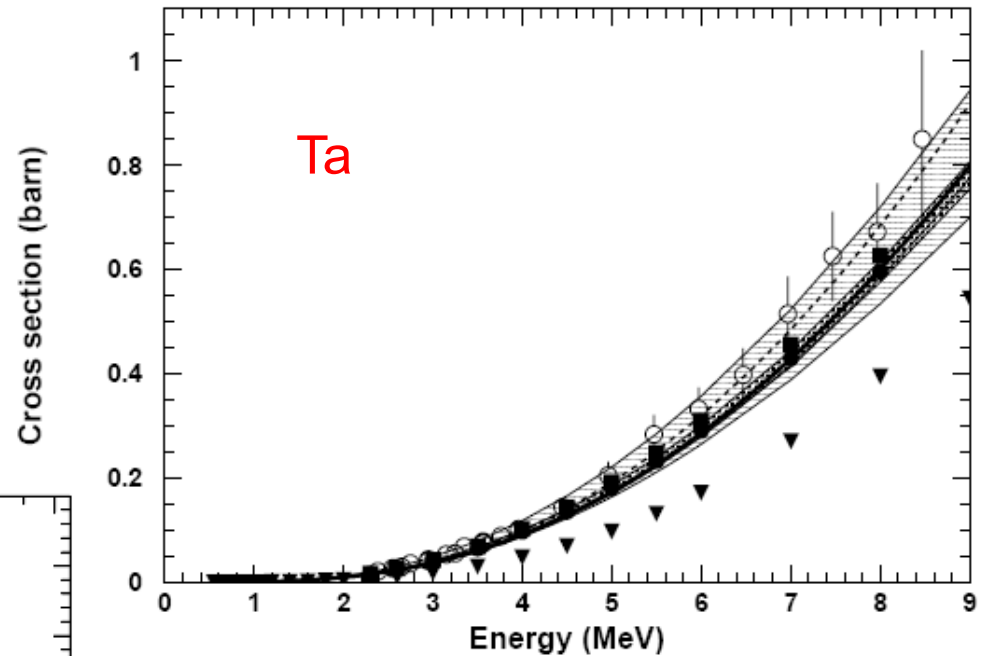
Thanks to RSICC!

*Theoretical cross  
sections tabulated by  
ISICS  
(thanks to S. Cipolla!)*

Subject to  
rigorous  
**experimental  
validation**

# Experimental validation, K shell

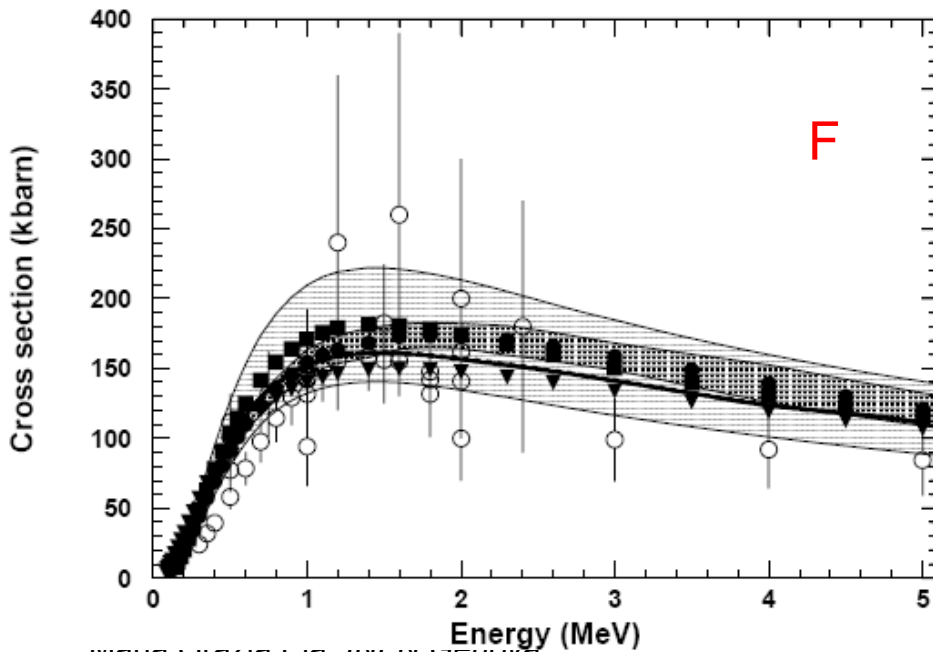
Experimental data from Paul & Sacher compilation



**Ionisation** cross sections

**X-ray production** cross sections

$$\sigma_i = \sigma_X / \omega_K$$





# K shell, protons

## $\chi^2$ test: p-values

One test case per element, for each  $\sigma$  model

Z	ECPSSR	ECPSSR HE	ECPSSR HS	ECPSSR UA	Paul Sacher	Kahoul et al.
6	0.200	0.203	0.490	0.200	0.998	0.989
7	0.057	0.061	0.246	0.057	0.818	0.806
8	0.906	0.910	0.922	0.906	0.981	0.971
9	0.147	0.136	0.124	0.147	0.029	0.012
10	0.044	0.046	0.083	0.044	0.791	0.171
60	0.296	0.185	0.550	0.296	0.385	< 0.001
62	0.049	0.029	0.642	0.049	0.570	< 0.001
65	0.322	0.161	0.928	0.322	0.310	0.523
67	< 0.001	< 0.001	0.844	< 0.001	0.012	0.001
69	0.003	0.004	0.078	0.003	0.741	< 0.001
73	0.013	0.002	0.946	0.013	0.193	0.998
90	< 0.001	< 0.001	0.001	< 0.001	< 0.001	< 0.001

P-VALUES FROM THE  $\chi^2$  TEST COMPARING K SHELL IONIZATION CROSS SECTIONS FOR PROTONS AGAINST EXPERIMENTAL DATA  $\sigma_{\alpha, X, A}$

Z	ECPSSR	ECPSSR HE	ECPSSR HS	ECPSSR UA	Paul Sacher	Kahoul et al.	Z	ECPSSR	ECPSSR HE	ECPSSR HS	ECPSSR UA	Paul Sacher	Kahoul et al.
6	0.797	0.818	0.959	0.797	< 0.001	< 0.001	40	0.045	0.066	0.102	0.039	0.208	0.044
7	< 0.001	< 0.001	0.063	< 0.001	< 0.001	< 0.001	41	0.002	0.003	0.002	0.002	< 0.001	< 0.001
8	0.989	0.989	0.989	0.986	< 0.001	< 0.001	42	0.998	1.000	0.999	0.998	1.000	0.682
9	0.793	0.774	0.724	0.793	0.296	0.005	45	< 0.001	< 0.001	< 0.001	< 0.001	< 0.001	0.001
10	1.000	1.000	0.999	1.000	< 0.001	< 0.001	46	0.991	0.989	0.992	0.991	0.930	0.626
12	0.069	0.069	0.497	0.023	0.053	< 0.001	47	0.507	0.724	0.668	0.504	0.027	0.008
13	0.011	0.001	0.052	0.005	< 0.001	< 0.001	48	< 0.001	< 0.001	< 0.001	< 0.001	< 0.001	0.700
14	0.015	0.015	0.033	0.015	< 0.001	0.035	49	< 0.001	< 0.001	< 0.001	< 0.001	< 0.001	< 0.001
15	0.709	0.705	0.611	0.709	0.802	0.615	50	0.967	0.964	0.975	0.967	0.961	0.001
16	0.798	0.797	0.713	0.798	0.940	0.699	51	0.930	0.941	0.966	0.930	0.997	0.088
17	0.661	0.668	0.741	0.661	0.239	0.737	53	0.032	0.066	0.011	0.032	0.034	0.005
18	0.396	0.427	0.805	0.599	0.784	0.999	55	0.323	0.242	0.470	0.323	0.624	0.281
19	0.993	0.993	0.988	0.993	0.990	0.978	56	0.295	0.137	0.916	0.295	0.852	0.001
20	0.032	0.021	0.124	0.032	0.007	0.067	57	0.053	0.035	0.163	0.053	0.297	0.003
21	0.280	0.357	1.000	0.280	0.992	< 0.001	58	0.136	0.120	0.715	0.136	0.966	0.033
22	0.207	0.234	0.234	0.204	0.824	< 0.001	59	0.038	0.047	0.033	0.038	0.135	0.760
23	0.003	0.005	0.147	0.003	0.023	< 0.001	60	0.267	0.163	0.638	0.267	0.659	< 0.001
24	0.397	0.471	0.852	0.366	0.743	0.014	64	0.336	0.391	0.297	0.336	0.024	0.019
25	0.424	0.435	0.532	0.293	0.739	0.477	65	0.273	0.123	0.944	0.273	0.025	0.116
26	0.975	0.975	0.588	0.921	0.960	0.990	67	0.024	0.002	0.996	0.024	0.151	0.003
27	0.970	0.981	0.981	0.966	0.994	0.202	69	0.115	0.142	0.043	0.115	0.238	0.006
28	0.234	0.349	0.554	0.140	0.514	0.086	70	< 0.001	0.009	< 0.001	< 0.001	0.125	0.041
29	0.674	0.765	0.890	0.530	0.987	< 0.001	72	0.394	0.436	0.773	0.394	0.997	0.612
30	0.998	0.998	0.992	0.996	0.999	0.004	73	0.043	0.031	0.007	0.043	0.511	0.953
31	0.046	0.081	0.394	0.046	0.376	0.293	74	0.401	0.533	< 0.001	0.401	0.666	0.025
32	0.002	0.005	0.153	0.001	0.228	0.374	75	0.139	0.167	0.130	0.139	0.253	0.268
33	0.073	0.114	0.411	0.073	0.618	0.685	78	0.163	0.164	0.670	0.163	0.907	0.833
34	0.415	0.487	0.632	0.418	0.978	0.978	79	0.071	0.343	< 0.001	0.071	0.999	0.161
35	< 0.001	0.307	0.326	0.265	0.300	0.005	82	0.019	0.353	< 0.001	0.019	0.026	< 0.001
36	0.243	0.329	0.531	0.243	0.806	0.994	83	0.371	0.353	0.751	0.371	0.849	0.356
37	0.104	0.118	0.147	0.104	0.149	0.007	90	0.028	0.013	< 0.001	0.028	< 0.001	< 0.001
38	< 0.001	0.001	0.001	< 0.001	0.005	0.158	92	0.936	0.931	0.997	0.936	0.805	< 0.001
39	0.112	0.124	0.192	0.112	0.798	0.784							

$\chi^2$  test: % test cases with p-value > 0.05

ECPSSR	ECPSSR rel.	ECPSSR-HS	ECPSSR-UA	Paul-Sacher	Kahoul
<b>All data</b>					
67	74	77	68	71	46
<b>Exclude higher energy data</b>					
69	75	86	69	70	48

## K shell

**ECPSSR with Hartree-Slater**  
correction best at **low energy**

**ECPSSR OK**

**High energy:** scarce  
measurements to really test  
ECPSSR rel.

*Conclusions based on  
objective, quantitative analysis*

Maria Grazia Pia, INFN Genova

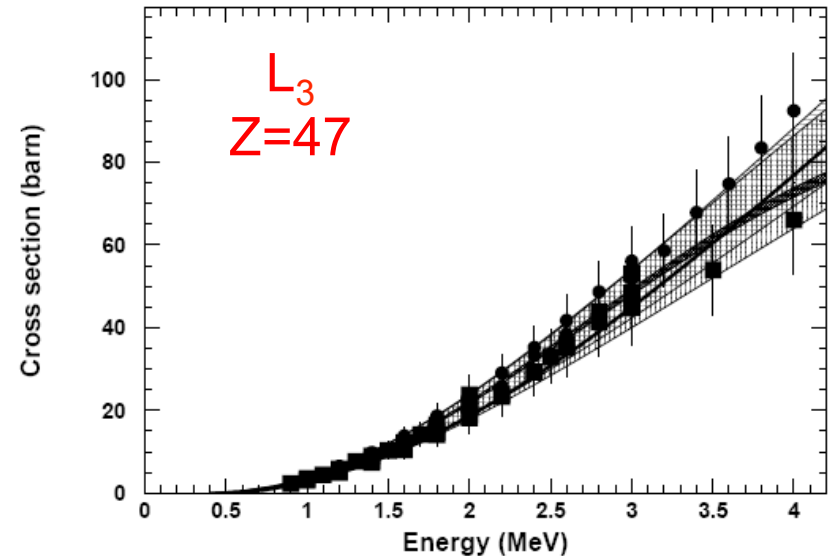
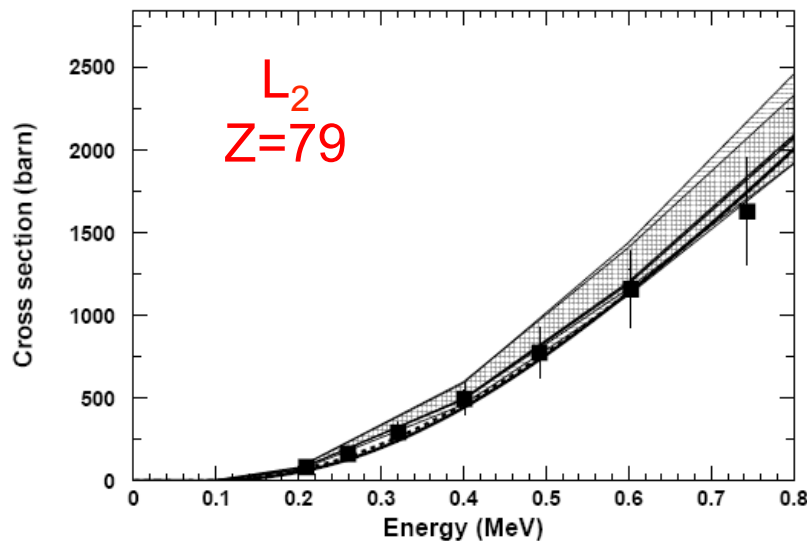
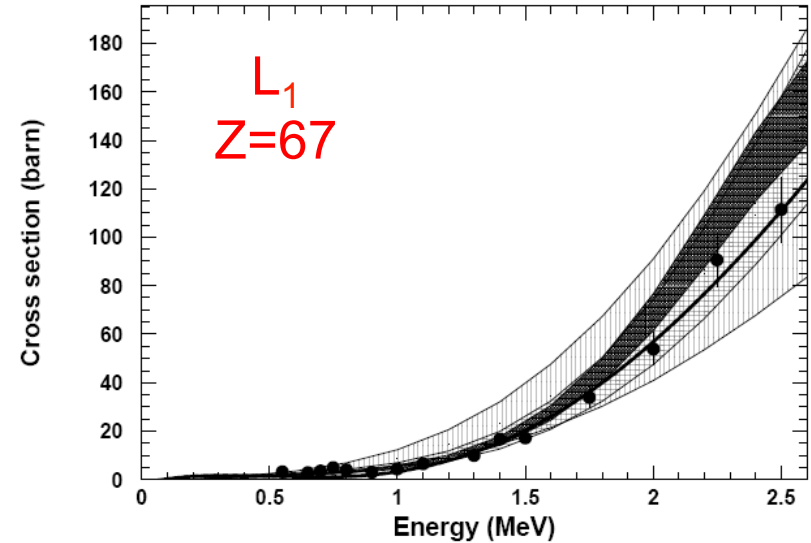
Contingency tables:  $\alpha = 0.05$

		$\chi^2$ test	ECPSSR	ECPSSR-HS
All data	Pass		44	50
	Fail		21	15
	p-value Fisher			0.327
	p-value Pearson $\chi^2$			0.240
	p-value Yates $\chi^2$			0.327
		$\chi^2$ test	ECPSSR	ECPSSR-HS
Exclude high E	Pass		44	55
	Fail		20	9
	p-value Fisher			0.034
	p-value Pearson $\chi^2$			0.020
	p-value Yates $\chi^2$			0.035
		$\chi^2$ test	Kahoul et al. ECPSSR-HS	
	Pass		30	50
	Fail		35	15
	p-value Fisher			0.001
	p-value Pearson $\chi^2$			< 0.001
	p-value Yates $\chi^2$			0.001

# Same validation process for L shell

## Experimental data

Compilations by  
Sokhi & Crumpton  
Orlic et al.  
Sow & Tang



# L shell

$\chi^2$  test: % with p-value > 0.05

	L <sub>1</sub>	L <sub>2</sub>	L <sub>3</sub>
<b>ECPSSR</b>	64	68	89
<b>ECPSSR UA</b>	64	79	89
<b>Miyagawa et al.</b>	26	78	85
<b>Orlic et al.</b>	41	70	56
<b>Sow et al.</b>	56	85	81

## **ECPSSR - United Atom**

best compatibility with  
experimental data

**ECPSSR OK**

**Orlic et al.:** worst compatibility  
with experimental data

## Contingency tables: $\alpha = 0.05$

$\chi^2$ test	ECPSSR-UA	ECPSSR
Pass	65	62
Fail	19	22
p-value Fisher	0.720	
p-value Pearson $\chi^2$	0.590	
p-value Yates $\chi^2$	0.719	

$\chi^2$ test	ECPSSR-UA	Miyagawa
Pass	65	51
Fail	19	30
p-value Fisher	0.060	
p-value Pearson $\chi^2$	0.043	
p-value Yates $\chi^2$	0.063	

$\chi^2$ test	ECPSSR-UA	Orlic
Pass	65	45
Fail	19	36
p-value Fisher	0.005	
p-value Pearson $\chi^2$	0.003	
p-value Yates $\chi^2$	0.005	

$\chi^2$ test	ECPSSR-UA	Sow
Pass	65	60
Fail	19	21
p-value Fisher	0.717	
p-value Pearson $\chi^2$	0.620	
p-value Yates $\chi^2$	0.754	

# M shell

The same analysis will be performed once adequate experimental data are available...


Collaboration with experimental groups is welcome

## Cross section data library ( $p$ , $\alpha$ )

Publicly distributed by **RSICC** and **NEA**

[RSICC Home Page](#)

RSICC DATA PACKAGE DLC-246





- 1. NAME AND TITLE OF DATA LIBRARY**  
PIXE2010: Proton/alpha Ionization (K, L, M shell), Tabulated Cross Section Library.
- 2. NAME AND TITLE OF DATA RETRIEVAL PROGRAMS:**  
IONXSEC: auxiliary software to print out data.
- 3. CONTRIBUTORS:**  
INFN, Sez. Genova, Italy; Max-Planck-Institut f. extraterrestrische Physik and MPI Halbleiterlabor, Germany; Creighton University, Illinois, USA; CNES, Toulouse, France; INFN, Laboratori Nazionali di Frascati, Italy; Berkeley University, USA; and Jožef Stefan Institute, Ljubljana, Slovenia

<http://www-rsicc.ornl.gov/codes/dlc/dlc2/dlc-246.html>


### Theoretical calculations (ISICS)

- PWBA
- ECPSSR
- ECPSSR – United Atom
- ECPSSR – Hartree-Slater
- ECPSSR – relativistic



NEA search engine  Go 

Data Bank > Computer program services

**NEA-1868 ZZ-PIXE2010.** last modified: 28-OCT-2011 | catalog | categories | new | search |  RSS

**ZZ PIXE2010, Proton/Alpha Ionization (K,L,M shell) Tabulated Cross-Section Library**

NAME OR DESIGNATION, COMPUTER, DESCRIPTION, METHODS, RESTRICTIONS ON THE COMPLEXITY OF THE PROBLEM, STATUS, REFERENCES, HARDWARE REQUIREMENTS, LANGUAGE, NAME AND ESTABLISHMENT OF AUTHORS, MATERIAL, CATEGORIES

**1. NAME OR DESIGNATION:** ZZ-PIXE2010 [ top ]

**2. COMPUTERS** [ top ]

To submit a request, click below on the link of the version you wish to order. Only liaison officers are authorised to submit online requests. Rules for requesters are available here.

Program name	Package id	Status	Status date
ZZ-PIXE2010	NEA-1868/01	Tested	28-OCT-2011

Machines used:

Package ID	Orig. computer	Test computer
NEA-1868/01	Many Computers	PC Windows

### Fitted, K shell

- Paul & Sacher ( $p$ )
- Kahoul et al. ( $p$ )
- Paul & Bolik ( $\alpha$ )

### Fitted, L shell

- Miyagawa et al.
- Sow et al.
- Orlic et al.

<http://www.oecd-nea.org/tools/abstract/detail/nea-1868/>

# Which ECPSSR calculator?

W. Brandt and G. Lapicki, “Energy-loss effect in inner-shell Coulomb ionization by heavy charged particles,” *Phys. Rev. A*, vol. 23, pp. 1717–1729, 1981

## ● **ISICS (C) (C++)**

- Z. Liu and S. J. Cipolla, “ISICS: A program for calculating K-, L- and M-shell cross sections from ECPSSR theory using a personal computer,” *Comp. Phys. Comm.*, vol. 97, no. 3, pp. 315–330, 1996
- and following updates

## ● **ERCS08 (FORTRAN)**

- V. Horvat, “ERCS08: A FORTRAN program equipped with a Windows graphics user interface that calculates ECPSSR cross sections for the removal of atomic electrons,” *Comp. Phys. Comm.*, vol. 180, no. 6, pp. 995–1003, 2009.

## ● **Z. Šmit’s code KIO/LIO (FORTRAN)**

- Z.Šmit, “K-shell ECPSSR cross sections for analytical applications,” *NIM. B*, vol. 36, no. 3, pp. 254–258, 1989
- Code kindly provided by the author

IEEE TRANSACTIONS ON NUCLEAR SCIENCE, VOL. 58, NO. 6, DECEMBER 2011

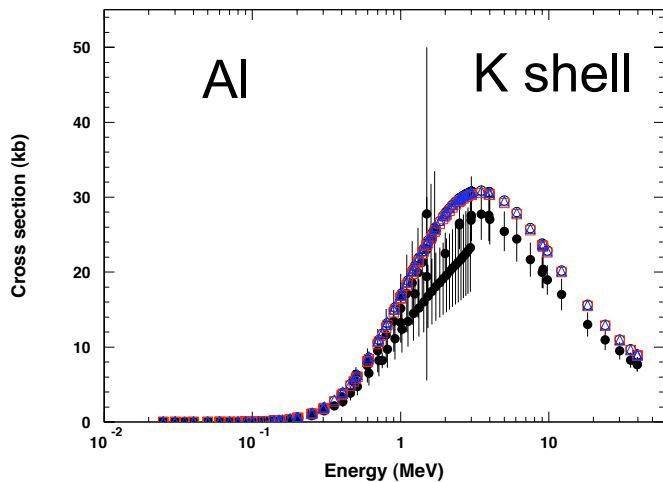
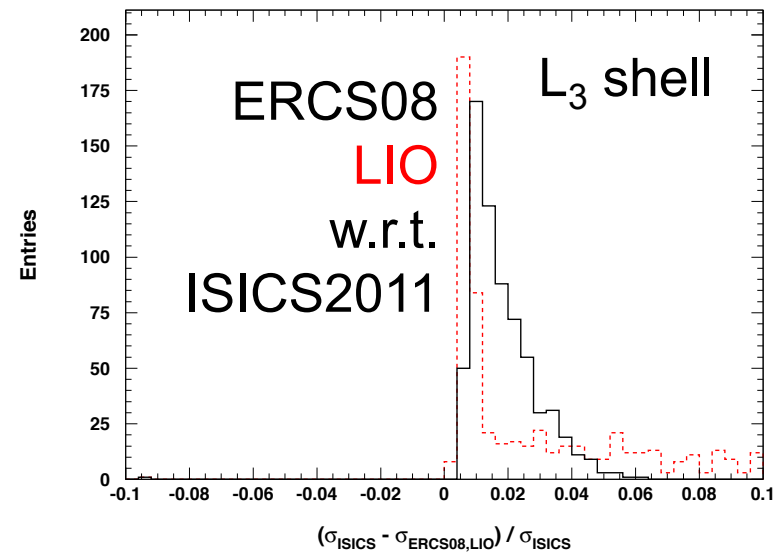
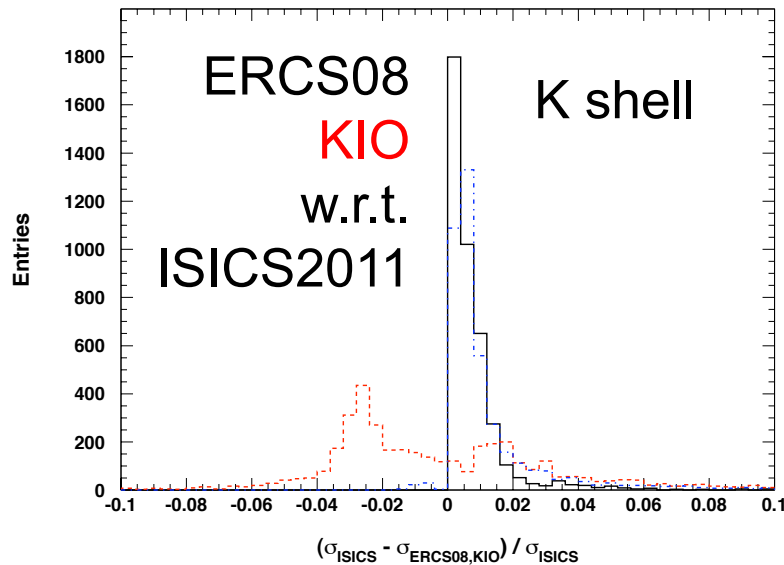
3269

Validation of Proton Ionization Cross Section  
Generators for Monte Carlo Particle Transport

Matej Batič, Maria Grazia Pia, and Paolo Saracco

**Relative comparison to experimental data**

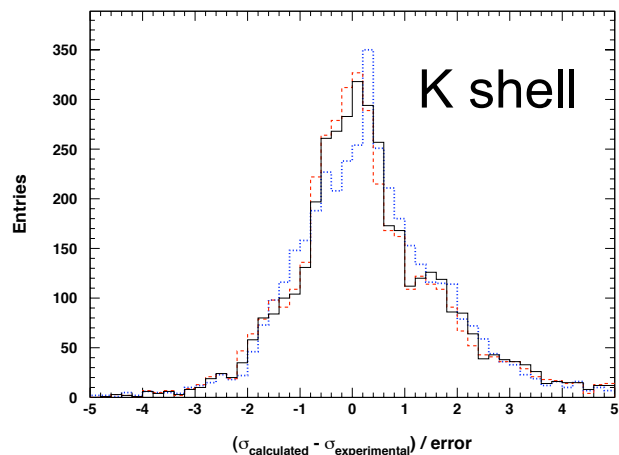
# Quantification of relative accuracy



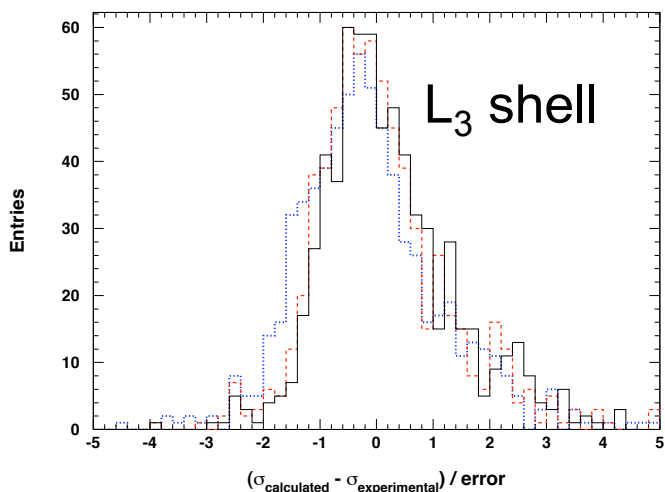
- $\chi^2$  test of compatibility with experiment over individual elements, for each calculator
- Pass/fail:  $\alpha = 0.05$
- Categorical analysis to compare compatibility with experiment
  - Fisher's exact test,  $\chi^2$  test



# Statistical analysis



Number of standard deviations w.r.t. experiment



Maria Grazia Pia, *INFN Genova*

$\chi^2$ test	ISICS 2011	ERCS08
K shell	Pass	51
	Fail	15
p-value Fisher	1	
p-value Pearson $\chi^2$	1	
p-value Yates $\chi^2$	0.835	

$\chi^2$ test	ISICS 2011	KIO
K shell	Pass	47
	Fail	19
p-value Fisher	0.551	
p-value Pearson $\chi^2$	0.426	
p-value Yates $\chi^2$	0.550	

## Statistically equivalent accuracy

$\chi^2$ test	ISICS 2011	ERCS08
L shell	Pass	66
	Fail	18
p-value Fisher	1	
p-value Pearson $\chi^2$	1	
p-value Yates $\chi^2$	0.835	

$\chi^2$ test	ISICS 2011	LIO
L shell	Pass	58
	Fail	26
p-value Fisher	0.161	
p-value Pearson $\chi^2$	0.219	
p-value Yates $\chi^2$	0.160	

# ISICS reengineering

Computer Physics Communications 183 (2012) 398–404



Contents lists available at SciVerse ScienceDirect

Computer Physics Communications

[www.elsevier.com/locate/cpc](http://www.elsevier.com/locate/cpc)



ISICSoo: A class for the calculation of ionization cross sections from ECPSSR and PWBA theory ☆

Matej Batič<sup>a,b,\*</sup>, Maria Grazia Pia<sup>a</sup>, Sam J. Cipolla<sup>c</sup>

<sup>a</sup> Istituto Nazionale di Fisica Nucleare, Sezione di Genova, Via Dodecaneso 33, 16146 Genova, Italy

<sup>b</sup> Jožef Stefan Institute, Jamova 39, 1000 Ljubljana, Slovenia

<sup>c</sup> Physics Department, Creighton University, Omaha, NE 68178, USA

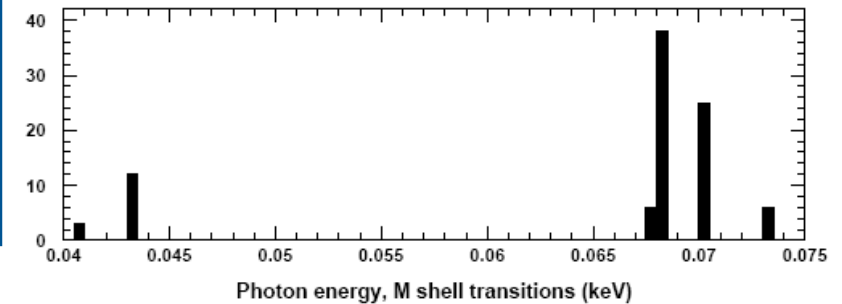
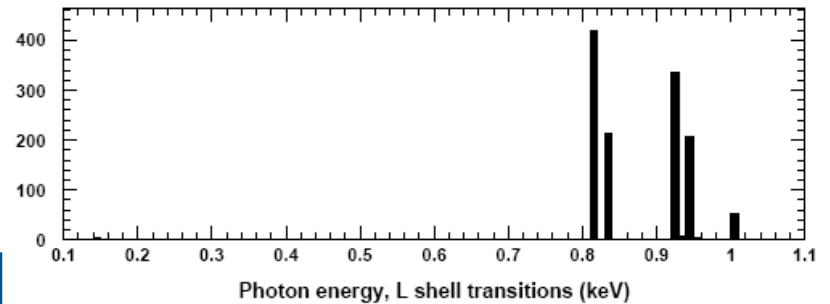
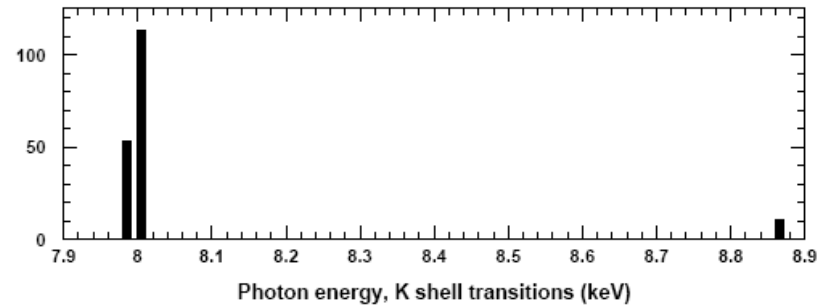
ISICS reengineered into a C++ class  
Can be used as a component in other systems

*Generated improvements to ISICS Windows version*

# Geant4 atomic relaxation

Geant4 simulation based on **EADL**

Validation of **X-ray energies**  
against Des Lattes et al.  
experimental review compilation



**2007**

IEEE TRANSACTIONS ON NUCLEAR SCIENCE, VOL. 54, NO. 3, JUNE 2007

## Geant4 Atomic Relaxation

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

594

IEEE TRANSACTIONS ON NUCLEAR SCIENCE, VOL. 54, NO. 3, JUNE 2007

## Validation of Geant4 Atomic Relaxation Against the NIST Physical Reference Data

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

# Atomic Binding Energies

- Bearden and Burr
- Carlson
- EADL
- Sevier (1979) *used by GUPIX*
- Table of Isotopes, 7<sup>th</sup> edition (1978): Shirley + Uppsala Group
- Table of Isotopes, 8<sup>th</sup> edition (1996): Larkins
- Williams (*X-ray Data Booklet, CRC Handbook*)

3246

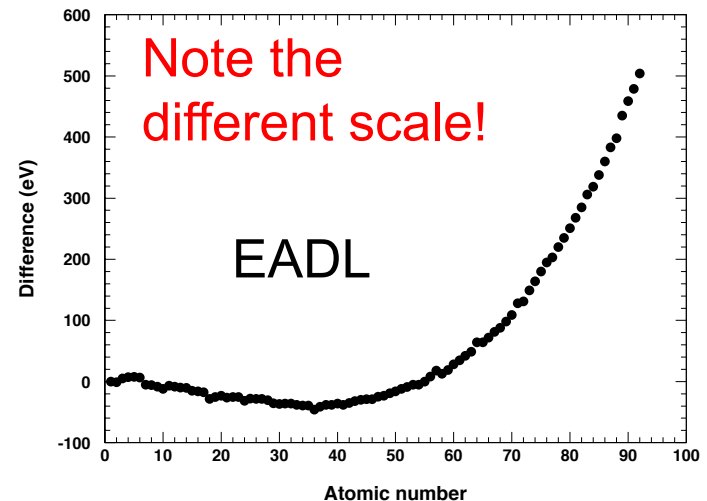
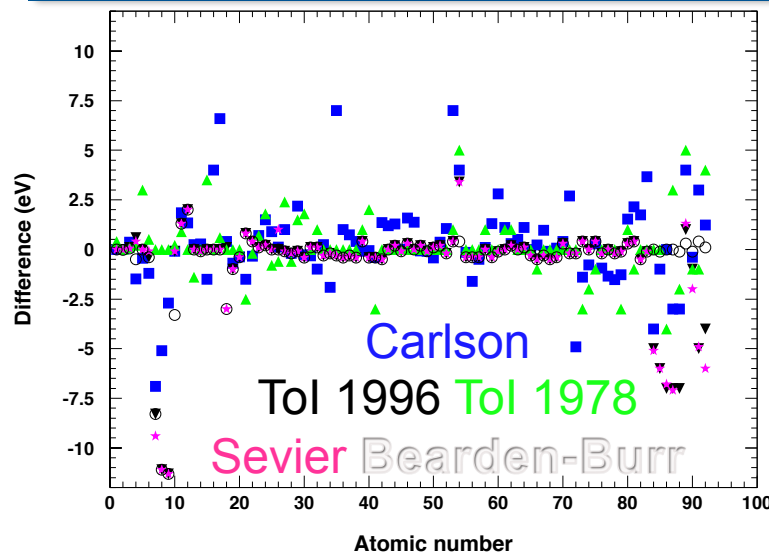
IEEE TRANSACTIONS ON NUCLEAR SCIENCE, VOL. 58, NO. 6, DECEMBER 2011

2011

Evaluation of Atomic Electron Binding Energies  
for Monte Carlo Particle Transport

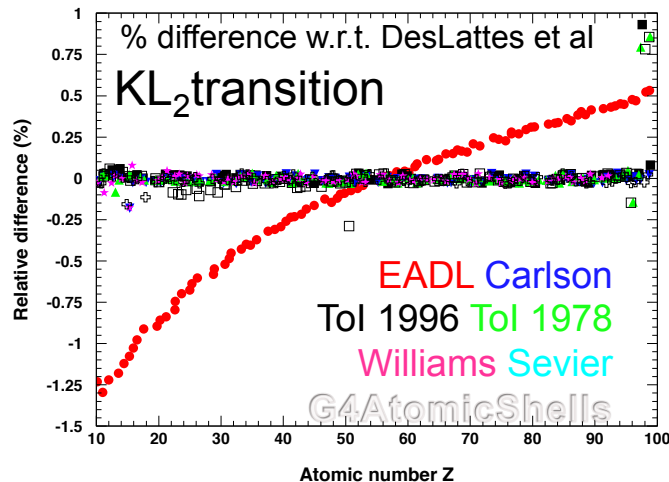
Maria Grazia Pia, Hee Seo, Matej Batic, Marcia Begalli, Chan Hyeong Kim, Lina Quintieri, and Paolo Saracco

## Difference w.r.t. Williams' binding energies



# Do they make any difference?

## X-ray energies



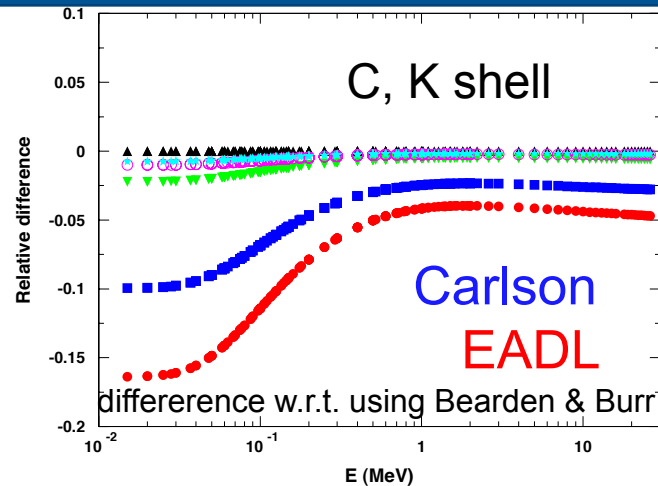
Compilation	K	L <sub>1</sub>	L <sub>2</sub>	L <sub>3</sub>	K+L	Fraction
Bearden and Burr	10	12	11	11	44	0.92 ± 0.04
Carlson	7	11	11	9	38	0.79 ± 0.06
EADL	8	4	1	3	16	0.33 ± 0.07
Sevier 1979	10	9	12	9	40	0.83 ± 0.05
Tol 1978	7	11	8	9	35	0.76 ± 0.06
Tol 1996	9	12	11	12	44	0.92 ± 0.04
Williams	8	12	11	9	40	0.85 ± 0.05

t-test for no mean difference,  $\alpha = 0.05$

$\chi^2$ test	Tol 1996	EADL
Pass	44	16
Fail	4	32
p-value Fisher	<0.0001	
p-value Yates $\chi^2$	<0.0001	

**statistically significant**  
**← EADL →**  
**inaccuracy**

## p impact ionisation $\sigma_{\text{ECPSSR}}$

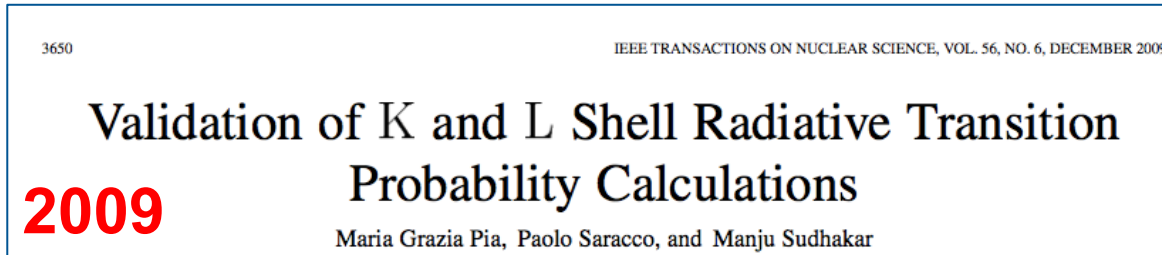


Compilation	Fraction
Bearden and Burr	0.76 ± 0.05
Carlson	0.76 ± 0.05
EADL	0.58 ± 0.06
Sevier 1979	0.76 ± 0.05
Tol 1978	0.78 ± 0.05
Tol 1996	0.76 ± 0.05
Williams	0.78 ± 0.05

$\chi^2$  test w.r.t. experiment,  $\alpha = 0.05$

$\chi^2$ test	Bearden-Burr	EADL
Pass	51	39
Fail	16	28
p-value Fisher		0.042
p-value Pearson $\chi^2$		0.027
p-value Yates $\chi^2$		0.043

# Radiative transition probabilities



## Hartree-Slater (*EADL*) vs. Hartree-Fock calculation methods

Comparison with experimental data

$\chi^2$ test % test cases with p-value > 0.05		
$\chi^2$ test	Hartree-Slater	Hartree-Fock
Pass	8	16
Fail	9	1
p-value Fisher		0.007
p-value Yates $\chi^2$		0.003

Transition probabilities calculated with Hartree-Fock methods are significantly more accurate

# eROSITA shielding optimization

Nuclear Instruments and Methods in Physics Research A 624 (2010) 321–329



Contents lists available at ScienceDirect

Nuclear Instruments and Methods in  
Physics Research A

journal homepage: [www.elsevier.com/locate/nima](http://www.elsevier.com/locate/nima)



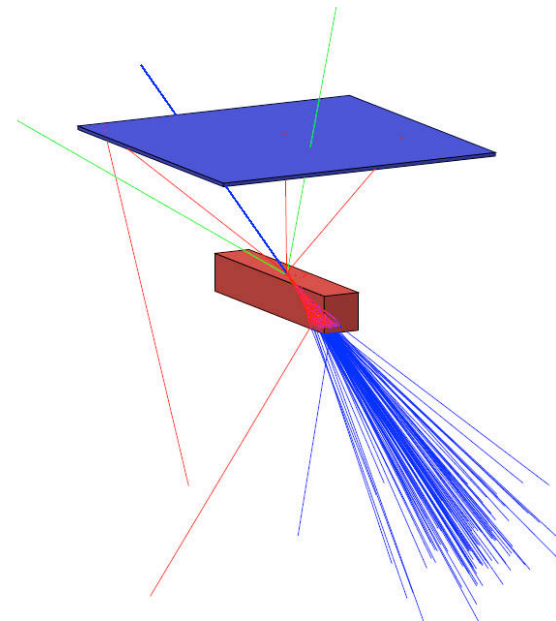
## Development of the focal plane PNCCD camera system for the X-ray space telescope eROSITA

Norbert Meidinger<sup>a,c,\*</sup>, Robert Andritschke<sup>a,c</sup>, Stefanie Ebermayer<sup>a,c</sup>, Johannes Elbs<sup>a,c</sup>, Olaf Hälker<sup>a,c</sup>, Robert Hartmann<sup>b,c</sup>, Sven Herrmann<sup>a,c</sup>, Nils Kimmel<sup>a,c</sup>, Gabriele Schächner<sup>a,c</sup>, Florian Schopper<sup>a,c</sup>, Heike Soltau<sup>b,c</sup>, Lothar Strüder<sup>a,c</sup>, Georg Weidenspointner<sup>a,c</sup>

<sup>a</sup> Max-Planck-Institut für extraterrestrische Physik, Giessenbachstrasse, 85748 Garching, Germany

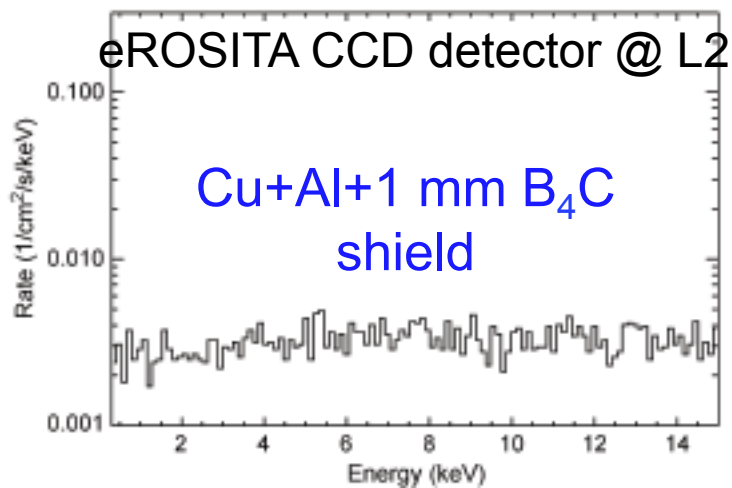
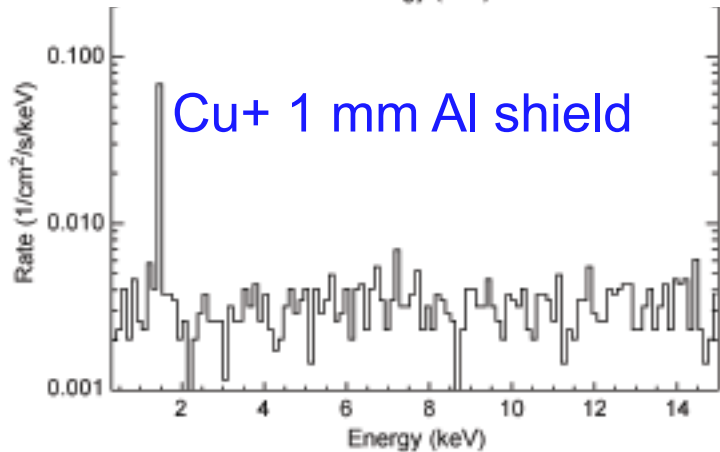
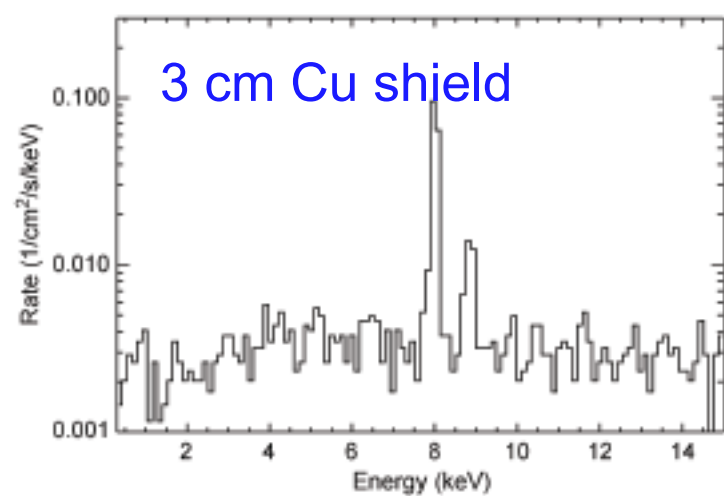
<sup>b</sup> PNSensor GmbH, Römerstrasse 28, 80803 München, Germany

<sup>c</sup> MPI Halbleiterlabor, Otto-Hahn-Ring 6, 81739 München, Germany



<http://www.ge.infn.it/geant4/physics/pixe/erosita.html>

## Geant4 advanced example



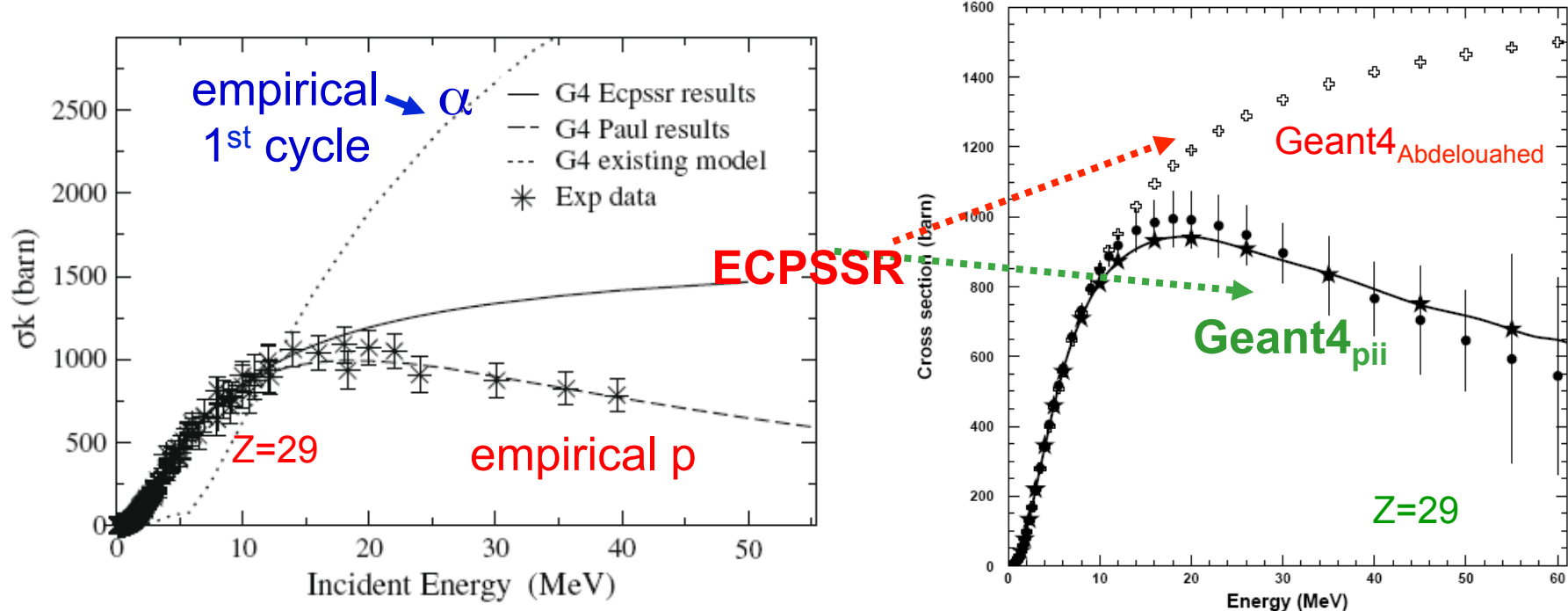
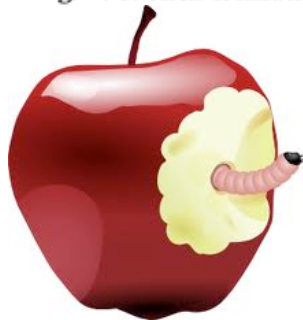


Fig. 2. K-shell ionization cross section by protons impact of element  $Z_2 = 29$ .



## New Geant4 cross section models for PIXE simulation

H. Ben Abdelouahed<sup>a,\*</sup>, S. Incerti<sup>b</sup>, A. Mantero<sup>c</sup>

Nuclear Instruments and Methods in Physics Research B 267 (2009) 37–44

MATERIALS CHARACTERIZATION 61 (2010) 59–64

available at [www.sciencedirect.com](http://www.sciencedirect.com)

ScienceDirect  
[www.elsevier.com/locate/matchar](http://www.elsevier.com/locate/matchar)

ELSEVIER

PIXE analysis of medieval silver coins **GUPIX**

H. Ben Abdelouahed<sup>a,\*</sup>, F. Gharbi<sup>b</sup>, M. Roumié<sup>b</sup>, S. Baccouche<sup>a</sup>, K. Ben Romdhane<sup>c</sup>, B. Nsouli<sup>b</sup>, A. Trabelsi<sup>a</sup>

<sup>a</sup> Centre National des Sciences et Technologies Nucléaires (CNSTN), Pôle technologique, 2020 Sidi Thabet, Tunis, Tunisia  
<sup>b</sup> ISEA Laboratory, Lebanese Atomic Energy Commission, National Council for Scientific Research, 11-8261, Beirut, Lebanon  
<sup>c</sup> Faculté des lettres et des sciences humaines, Université de Tunis, Tunisia

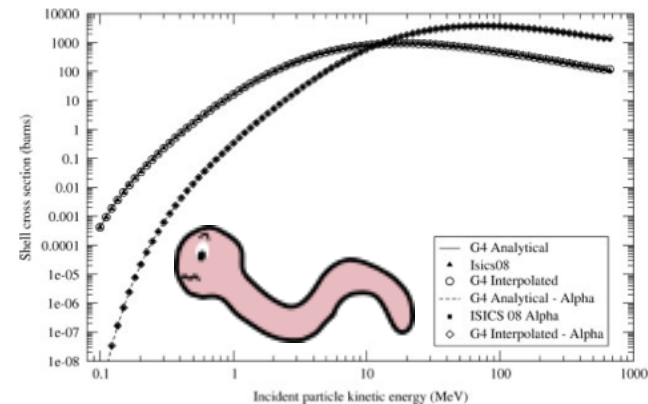
**Research Article** X-RAY spectrometry

Received: 3 September 2010 Revised: 11 January 2011 Accepted: 13 January 2011 Published online in Wiley Online Library: 24 March 2011

(wileyonlinelibrary.com) DOI 10.1002/xrs.1301

### PIXE simulation in Geant4

A. Mantero,<sup>a,\*</sup> H. Ben Abdelouahed,<sup>b</sup> C. Champion,<sup>c</sup> Z. El Bitar,<sup>d</sup> Z. Francis,<sup>e</sup> P. Guèye,<sup>f</sup> S. Incerti,<sup>g</sup> V. Ivanchenko,<sup>h,i,j</sup> and M. Maire<sup>i,k</sup>





# In my end is my beginning...

*T.S. Eliot, East Coker*

## Geant4 provides functionality for PIXE simulation

Rigorous, quantitative validation of all the physics components  
specific to PIXE simulation

The software is adequate for experimental applications concerned with  
**relative effects** of **experimentally relevant** spectra

Successfully used for eROSITA shielding optimisation

Conceptual issues of condensed-discrete transport are being investigated

## Collaboration is welcome!

<http://cern.ch/geant4/>

<http://www.ge.infn.it/geant4/>