Atomic data in Monte Carlo transport codes and their validation

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WANDA

Washington DC, 22-24 January 2019

10 minutes to highlight a few concepts and to introduce topics for discussion

A FISH CALLED WANDA out of water

Foreword

I am here because of →

2268 IEEE TRANSACTIONS ON NUCLEAR SCIENCE, VOL. 65, NO. 8, AUGUST 2018

First Assessment of ENDF/B-VIII and EPICS Atomic Data Libraries

Min Cheol Han, Maria Grazia Pia, Paolo Saracco, and Tullio Basaglia

and what is behind it… https://www.ge.infn.it/geant4/papers/index.html

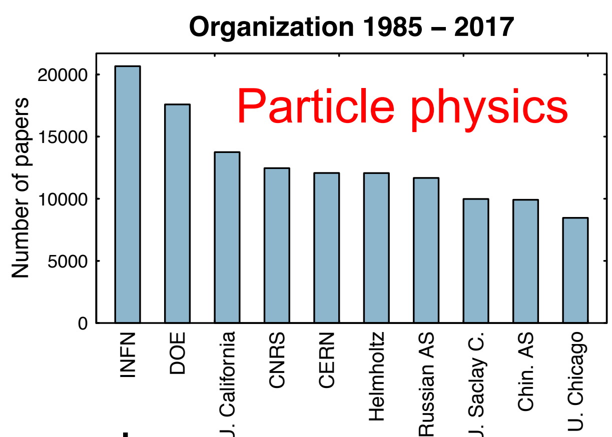
which is partly related to Geant 4 although my activity in this domain started even before GEANT 3 was born

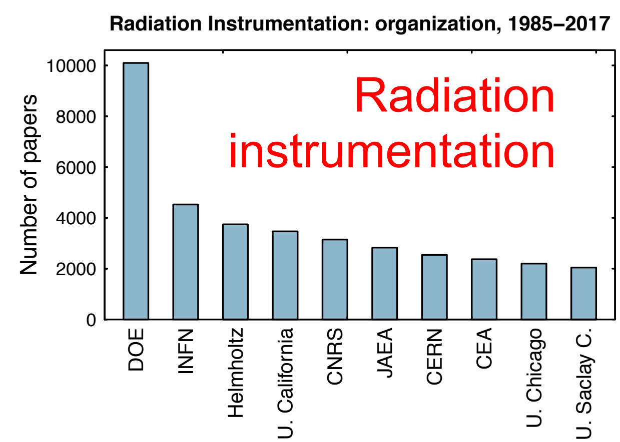
I am here thanks to the support of my institute: **INFN**

INFN is a very productive scientific organization!

NOT scaled by →

- population
- GDP
- expenditure for research





Source: Web of Science, Clarivate Analytics

Evaluated Atomic Libraries

Conventional designation for

- **EADL** (atomic) atomic parameters and relaxation
- **EEDL** (electron)
- **EPDL** (photon)

(EEDL, EPDL: interaction cross sections)

- **Originally released by LLL/LLNL** EADL, EEDL: 1991, EPDL: 1997
- Released in **ENDF/B** since version **VI.8**
- Released by **IAEA** as **EPICS** since 2014

Evaluated?

QED: precision calculations are feasible!

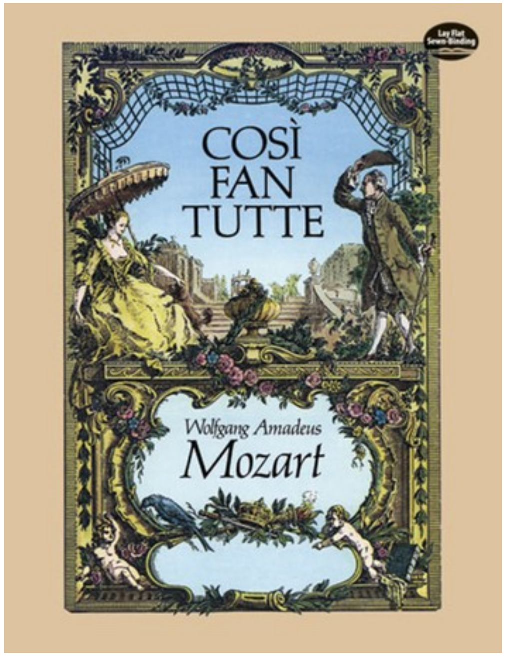
EEDL and **EPDL** are tabulations of **theoretical calculations**

The origin of **EADL** data is only partially known

- theoretical *(Scofield's and Chen's transition rates)*
- semi-empirical *(EPICS 2017 e^- binding energies)*
- undocumented *(several parameters)*

Besides EADL, EEDL, EPDL, several compilations/tabulations of electromagnetic parameters and cross sections are available

Mozart effect in Monte Carlo simulation



Electron-photon interaction modelling based on EADL/EEDL/EPDL started in RD44, was first released in Geant4 in 1999

Same approach later adopted for p/ion ionisation, PIXE

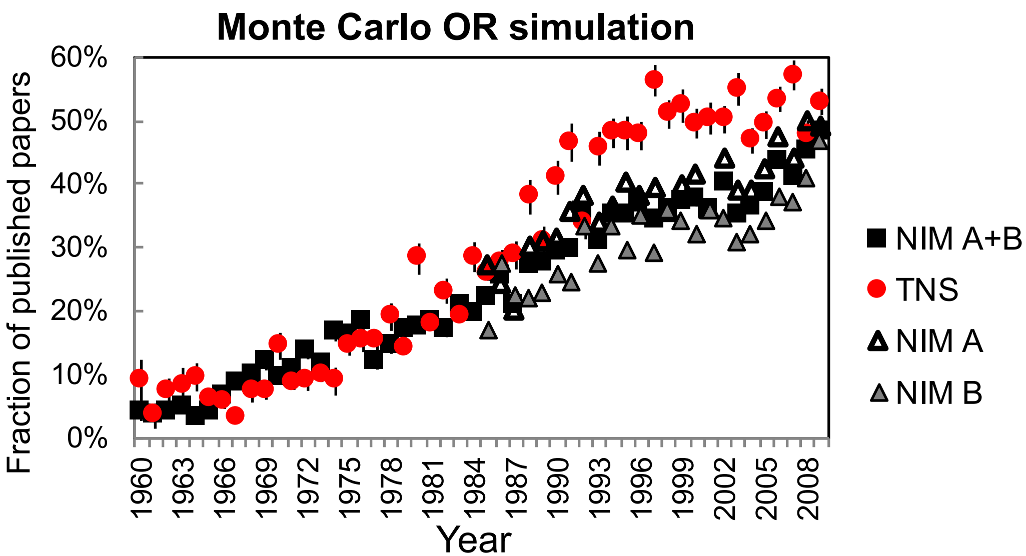
Initially ostracized by Geant4 more "conservative" electromagnetic folks,

then widely adopted by EGS, FLUKA, Geant4, MCNP, Penelope, PHITS…

- neglecting the intrinsic limitations of EADL/EEDL/EPDL (**IPA** and **IA**)
- overlooking the necessary [hard] work: validation tests
- forgetting the quest for state-of-the-art modelling in Monte Carlo transport

Electromagnetic physics modelling based on EADL/EEDL/EPDL
has been the key for the success of Geant4 outside the application domain
it was originally addressed to *(LHC experiments)*

Simulation pervades experimental activities related to nuclear/particle/astro/medical physics

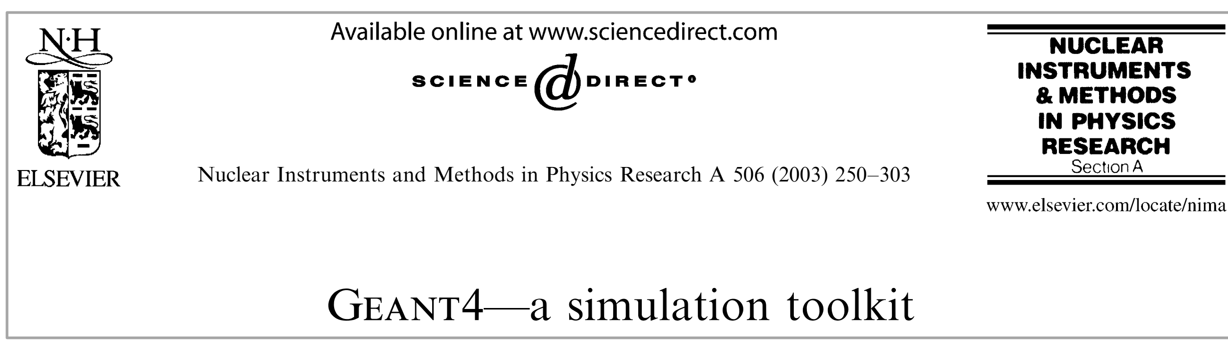


Fraction of publications in popular Nuclear Science & Technology journals since 1960

Most cited paper in

- Nuclear Science & Technology
- Instruments & Instrumentation
- Physics, Particles & Fields

Source: Web of Science, Clarivate Analytics



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Nuclear Instruments and Methods in Physics Research A 506 (2003) 250–303

NUCLEAR INSTRUMENTS & METHODS IN PHYSICS RESEARCH Section A

www.elsevier.com/locate/nima

GEANT4—a simulation toolkit

Not only EADL/EEDL/EPDL…

- Several compilations of atomic parameters
  - atomic binding energies by Bearden-Burr, Carlson *(used by Penelope)*, Williams *(X-ray Booklet),* Larkins et al. *(ToI)* etc.
  - Biggs et al. Hartree-Fock Compton profiles *(used by several MC codes)*
  - NIST ionisation energies
  - *etc.*
- Tabulations of interaction cross sections
  - Kissel's RTAB (photon elastic scattering)
  - ELSEPA: e^+ and e^- elastic scattering (Salvat-Jablonski-Powell)
  - Brennan and Cowan tables for X-ray calculations
  - Brunetti et al. library for X-ray–matter interaction cross sections
  - *etc.*
- Parameterisations of semi-empirical evaluations
  - e.g. Biggs-Lighthill *(used by Geant4 standard electromagnetic package)*

Which data represent the state of the art?

Do EADL/EEDL/EPDL reflect the state of the art?

State of the art: the best one can do, given the body of knowledge

"…data that I used to produce what I judge to be the BEST binding energies to use in EPICS2017"

D. E. Cullen, A survey of Atomic Binding energies for use **in EPICS 2017**, IAEA-NDS-224, Sep. 2017

2722 IEEE TRANSACTIONS ON NUCLEAR SCIENCE, VOL. 47, NO. 6, DECEMBER 2000

Comparative Evaluation of Photon Cross-Section Libraries for Materials of Interest in PET Monte Carlo Simulations

Habib Zaidi

"The cross-section values produced by the LLNL […] **are thought to be** the most up-to-date and **accurate** coefficients available"

Contents lists available at ScienceDirect

Nuclear Instruments and Methods in Physics Research A

journal homepage: www.elsevier.com/locate/nima

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Validation of the Geant4 electromagnetic photon cross-sections for elements and compounds

G.A.P. Cirrone [a], G. Cuttone [a], F. Di Rosa [a], L. Pandola [b,*], F. Romano [a], Q. Zhang [a,c,**]

Comparison of theoretical calculations, **not validation!**

Only a small fraction of EADL, EEDL and EPDL data has been directly validated with respect to measurements

Some indirect validation through complex experimental observables
(e.g. measurements of energy deposition resulting from several physics processes + MC modelling)

Applied both to direct validation tests and to the validation of complex simulated observables

Validation method

Comparison of **physics observable** resulting from each physics model with **experimental measurements**

Goodness-of-fit tests

χ^2

Anderson-Darling

Cramer-von Mises

Kolmogorov-Smirnov

rejection of the null hypothesis in the set of test cases

Comparison of the **capability of physics models to reproduce experiment**

Analysis of **contingency tables**

χ^2

Fisher exact test

Barnard (Boschloo, Suissa-Shuster)

McNemar test

Objective identification of the **state of the art** to model the observable

A. Lechner, M. G. Pia, M. Sudhakar, Validation of Geant4 low energy electromagnetic processes against precision measurements of electron energy deposit, *IEEE Trans. Nucl. Sci.,* vol. 56, no. 2, pp. 398-416, 2009

New is ~~always~~ sometimes better

Scofield (1973) photoelectric cross sections exhibit significantly better compatibility with experiment than more recent relativistic calculations by **Chantler** (2000, available at NIST web site) and **Brennan-Cowan** data (1992, popular in photon science)

M. C. Han et al., "Validation of Cross Sections for Monte Carlo Simulation of the Photoelectric Effect", IEEE Trans. Nucl. Sci., vol. 63, no. 2, pp. 1117–1146, 2016

Electron impact ionisation cross sections, inner shells

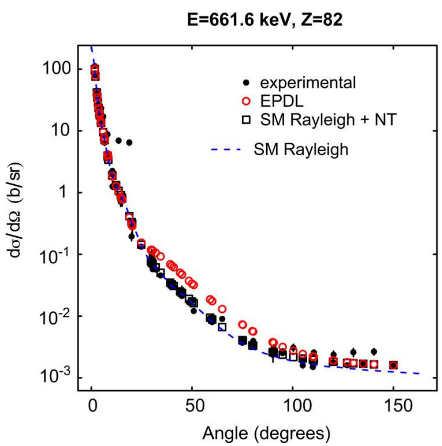
K shell: no significant difference in compatibility with experiment is observed between **EEDL** (1991) and Bote-Salvat (2008-2014) distorted-wave calculations

$L_{1,2,3}$ subshells: univocal conclusions limited by scarcity of experimental data

T. Basaglia et al., "Validation of Shell Ionization Cross Sections for Monte Carlo Electron Transport", IEEE Trans. Nucl. Sci., vol. 65, no. 8, pp. 2279–2302, 2018.

Old wine tastes better (sometimes)

AKA "it has been around for a long time, it must be right"
AKA "all MC codes use it, it must be right"



e.g. photon elastic scattering differential cross sections

Test		Penelope 2001	Penelope 2008-2011	EPDL	EPDL ASF	SM	RF	NF	MF	MF ASF	RF ASF
all	Test cases	71	71	71	71	71	71	71	71	71	71
	Pass	19	27	27	18	55	18	25	35	37	34
	Fail	52	44	44	53	16	53	46	36	34	37
	Efficiency	0.27	0.38	0.38	0.25	0.77	0.25	0.35	0.49	0.52	0.48
	Error	±0.05	±0.06	±0.06	±0.05	±0.06	±0.05	±0.06	±0.06	±0.06	±0.06
$\theta \leq 90°$	Test cases	67	67	67	67	67	67	67	67	67	67
	Pass	19	27	27	18	55	18	25	35	36	32
	Fail	48	40	40	49	12	49	42	32	31	35
	Efficiency	0.28	0.40	0.40	0.27	0.82	0.27	0.37	0.52	0.54	0.48
	Error	±0.05	±0.06	±0.06	±0.05	±0.05	±0.05	±0.06	±0.06	±0.06	±0.06
$\theta > 90°$	Test cases	17	17	17	17	17	17	17	17	17	17
	Pass	1	1	1	1	10	1	1	0	2	4
	Fail	16	16	16	16	7	16	16	17	15	13
	Efficiency	0.06	0.06	0.06	0.06	0.59	0.06	0.06	< 0.06	0.12	0.24
	Error	±0.06	±0.06	±0.06	±0.06	±0.12	±0.06	±0.06		±0.08	±0.10

S-matrix calculations based on RTAB (2000) exhibit significantly better compatibility with experiment than EPDL (1997) approach based on form factor approximation

M. Batič, et al., "Photon elastic scattering simulation: Validation and improvements to Geant4", *IEEE Trans. Nucl. Sci.*, vol. 59, no. 4, pp. 1636–1664, 2012.

Deutsch-Märk total electron ionisation cross sections (2005) exhibit significantly better compatibility with experiment than EEDL (1991) at low energies (< 1 keV)

H. Seo et al., "Ionization cross sections for low energy electron transport", *IEEE Trans. Nucl. Sci.*, vol. 58, no. 6, pp. 3219–3245, 2011.

(negative) **Improvements**

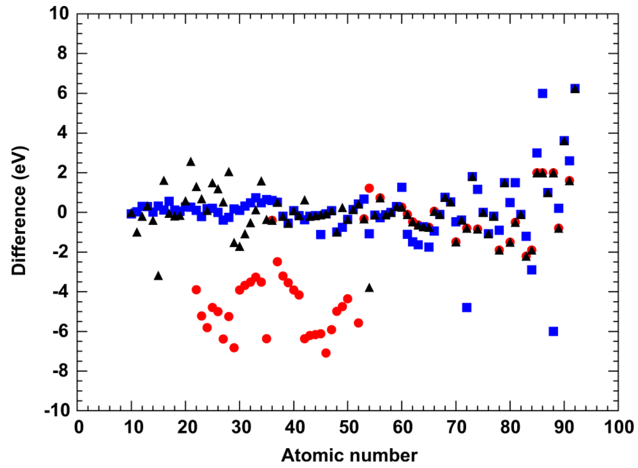


Fig. 37. KL_3 transition, difference between X-ray energies calculated from binding energies and experimental data from [64] versus atomic number: binding energies from *G4AtomicShells* (red circles), from Carlson (blue squares) and Williams (black triangles).

"Improved" Geant4 electron binding energies mix values from Carlson and Williams compilations, based on different reference levels *(vacuum level and Fermi level, respectively)*

Geant4 "improved" Biggs-Lighthill parameterisation coefficients of photoelectric cross sections result in worse compatibility with experiment than the original (1987) values

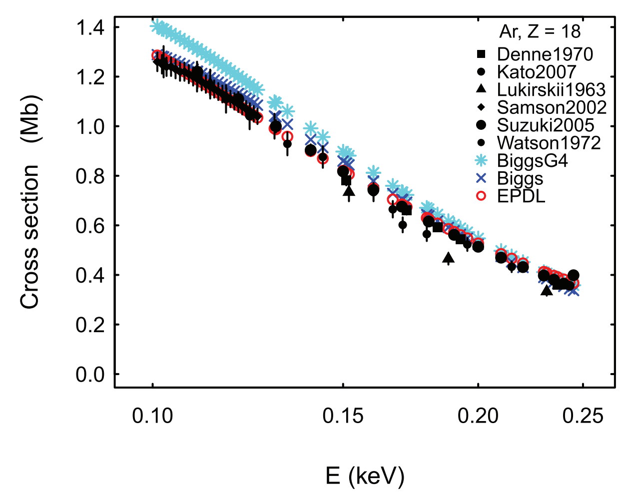


Fig. 28. Total photoionization cross section for argon as a function of photon energy, above 100 eV: original and modified Biggs-Lighthill parameterizations exhibit different behavior with respect to experimental data.

Food for thought

Software engineering

- Version control
- Configuration management
- Consistent distribution
  - unique source + mirrors?
- Release process (<u>documented</u>)
- Test process (<u>documented</u>)
- Suitable format for physics needs
- Documentation

Physics

- State of the art
- Validation
  - Sound epistemology, statistical tools, data
- Uncertainty quantification
- Multiple physics options?
- More extensive set of atomic parameters *consistency!*
- Protons, ions

International cooperation is necessary to address the wide and complex needs of atomic data for Monte Carlo simulation *(i.e. for nearly all basic and applied experimental nuclear/particle physics)*

We would like to see **some concrete steps to improve the current situation**

Our expertise can be a valuable contribution to common efforts