Meeting of the **WPEC Expert Group**
on the Recommended Definition of a
General Nuclear Database Structure (EG-GNDS)

Atomic Data

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WebEx meeting
12 May 2020

Foreword

Due to limited time allocation, mainly an introduction to topics for discussion

Geant4 “low energy” electromagnetic physics: based on EA/E/PDL, late ‘90s

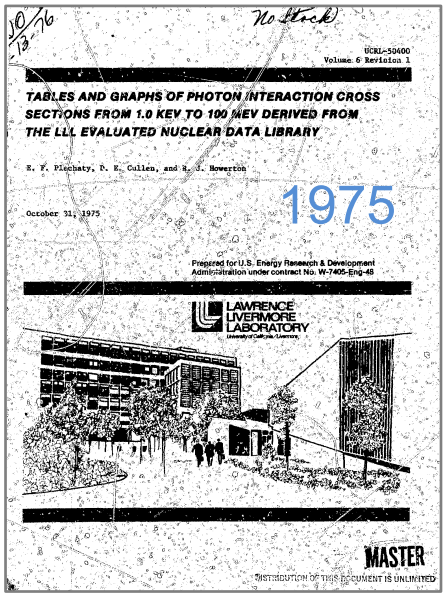
Background

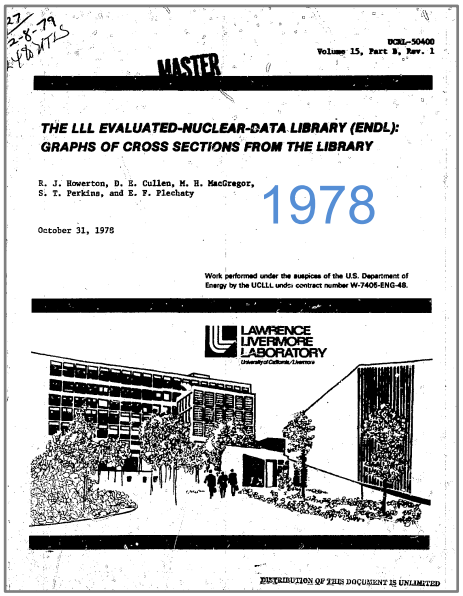
Rigorous statistical data analysis
Goodness-of-fit tests w.r.t. experimental data
+ categorical data analysis based on contingency tables

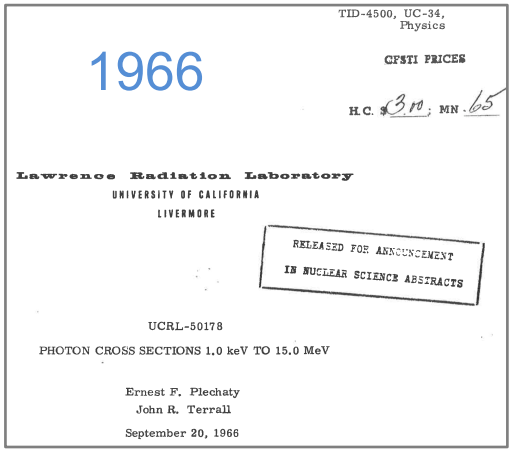
- T. Basaglia et al., “Evolutions in photoelectric cross section calculations and their validation”, *IEEE Trans. Nucl. Sci.,* vol. 67, no. 3, pp. 492-501, 2020.
- M. C. Han et al., “ First Assessment of ENDF/B-VIII and EPICS Atomic Data Libraries”, *IEEE Trans. Nucl. Sci.,* vol. 63, no. 8, pp. 2268-2278, 2018.
- T. Basaglia et al., “ Validation of Shell Ionization Cross Sections for Monte Carlo Electron Transport”, *IEEE Trans. Nucl. Sci.,* vol. 63, no. 8, pp. 2279-2302, 2018.
- 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.
- 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.
- H. Seo et al., “Ionization cross sections for low energy electron transport”, *IEEE Trans. Nucl. Sci.,* vol. 58, no. 6, pp. 3219–3245, 2011.
- M. G. Pia et al., “Evaluation of atomic electron binding energies for Monte Carlo particle transport”, *IEEE Trans. Nucl. Sci.,* vol. 58, no. 6, pp. 3246–3268, 2011.
- M. G. Pia et al., “Validation of K and L shell radiative transition probability calculations”, *IEEE Trans. Nucl. Sci.,* vol. 56, no. 6, pp. 3650–3661, 2009.
- S. Guatelli et al., “Validation of Geant4 Atomic Relaxation against the NIST Physical Reference Data”, *IEEE Trans. Nucl. Sci.,* vol. 54, no. 3, pp. 594-603, 2007.
- G. Weidenspointner et al., “Validation of Compton Scattering Monte Carlo Simulation Models”, *Proc. IEEE Nucl. Sci. Symp.,* 2013.
- M. Begalli et al., “Validation of Geant4 Electron Pair Production by Photons”, *Proc. IEEE Nucl. Sci. Symp.,* 2013.

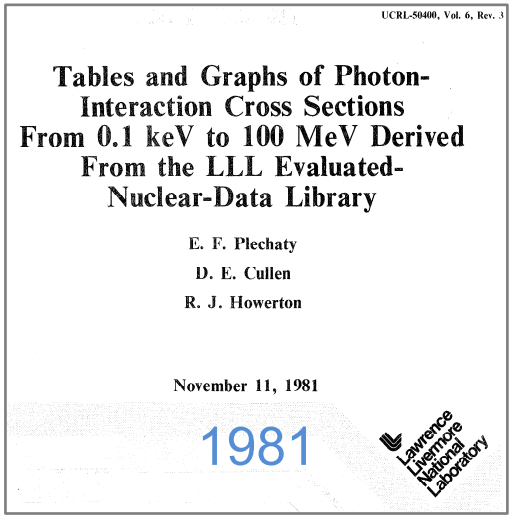
Evaluated Atomic Libraries

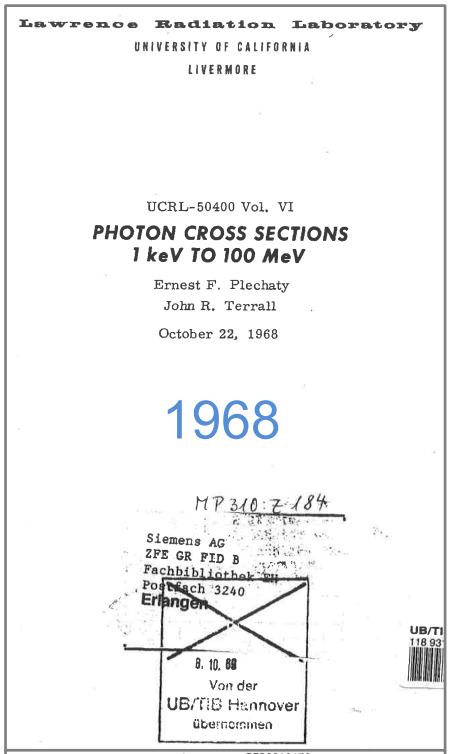
- **EADL** (atomic) **1991**
- **EEDL** (electron) **1991**
- **EPDL** (photon) **1997**

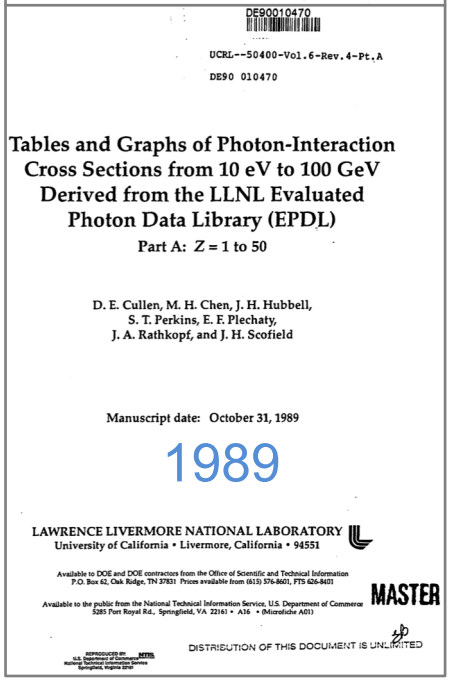












- **Originally released by LLL/LLNL**
- Released in **ENDF/B** since version **VI.8**
- Released by **IAEA** as **EPICS** since 2014

Formats:
ENDL
ENDF

The world changes…

…but the atomic E✳DL have not changed much since the ‘60s

Originally photons only
Motivated by nuclear engineering use

Nowadays, directly or indirectly used by all major Monte Carlo codes in scientific research and engineering applications, and by other specialized computational tools

User requirements, physics modelling approaches, computational methods have significantly evolved in the past decades

EADL/EEDL/EPDL
de facto **orphan** for >10 years

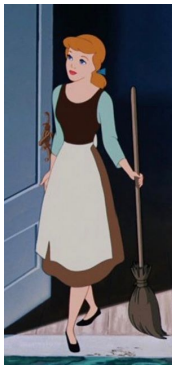
M. C. Han et al., “ First Assessment of ENDF/B-VIII and EPICS Atomic Data Libraries”, *IEEE Trans. Nucl. Sci.*, vol. 63, no. 8, pp. 2268-2278, 2018.

Atomic data and GNDS

A format should serve the data. *Which data?*

Atomic parameters	Molecular? Parameters propaedeutic to model electromagnetic interactions in particle transport codes
Electron/photon interactions	Any additional processes Any additional data Any different computational approaches
	w.r.t. current EEDL/EPDL?
Positrons **Protons/hadrons** **Ions**	Neglected in ENDF atomic data libraries Needed by particle transport codes Some data compilations exist

Does GNDS serve atomic data?



ENDF data translation

Probably ~**OK**
(quick glance at the documentation, should be systematically verified)

A more modern approach to atomic data libraries would be beneficial to better reflect current user needs and to foresee future perspectives *(research, rather than just service!)*

A **roadmap**
for the data
and
for **GNDS**

⓪ ENDF data

❶ ENDL data

❷ Atomic parameters and electron/photon data currently used in transport codes

❸ New electron/photon data assessed as state of the art

❹ Data extensions and improvements

Problem domain decomposition!

GNDS documentation about electron ionization:

"It is assumed that both the scattered and the recoil electrons continue in the direction of the incident electron, and that no kinetic energy is transferred to the residual atom".

A format standard should be **agnostic** to physics modelling assumptions and data content

BUT transparency is a requirement for physics data libraries to be used in scientific environments

We want the data content, origin, assumptions etc. to be documented

Metadata: to be defined to enrich the raw data with additional information to identify and characterize them

ENDL data

EADL/EEDL/EPDL content is different in ENDF and ENDL format

EADL CONTENT

Physics Data	EADL91		EPICS2014		EPICS2017	
	ENDL	ENDF-6	ENDL	ENDF-6	ENDL	ENDF-6
Number of electrons	yes	yes	yes	yes	yes	yes
Binding energy	yes	yes	yes	yes	yes	yes
Kinetic energy	yes	-	yes	-	yes	-
Average radius	yes	-	yes	-	yes	-
Radiative level width	yes	-	yes	-	yes	-
Non-radiative level width	yes	-	yes	-	yes	-
Average energy to the residual atom per initial vacancy	yes	-	yes	-	yes	-
Average energy of particles per initial vacancy	yes	-	yes	-	yes	-
Average number of particles per initial vacancy	yes	-	yes	-	yes	-
Radiative transition probability and emitted particle energy	yes	yes	yes	yes	yes	yes
Non-radiative transition probability and emitted particle energy	yes	yes	yes	yes	yes	yes

GNDS Consider encoding atomic parameters present in ENDL format

Caveat Some parameters present in previous EADL versions have disappeared in EPICS 2017

The origin of many of these parameters is unknown (undocumented)

Requirement: metadata to document the origin etc.

Data known to be useful

- Some atomic data compilations, not currently included in EADL/EEDL/EPDL, have been used in Monte Carlo particle transport codes for a long time
  - e.g. Biggs' Compton profiles to model Doppler broadening in Compton scattering
  - e.g. probability of creating a vacancy in an atomic shell in Compton scattering
- Survey of atomic parameters and electron/photon data in particle transport codes
- Encoding in GNDS
  - Possible with existing definitions?
  - Need GNDS extensions?

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

State of the art: the best one can do with the existing body of knowledge

Validation

of physics content
(e.g. cross sections)

of composite observables
(e.g. energy deposition in a detector)

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

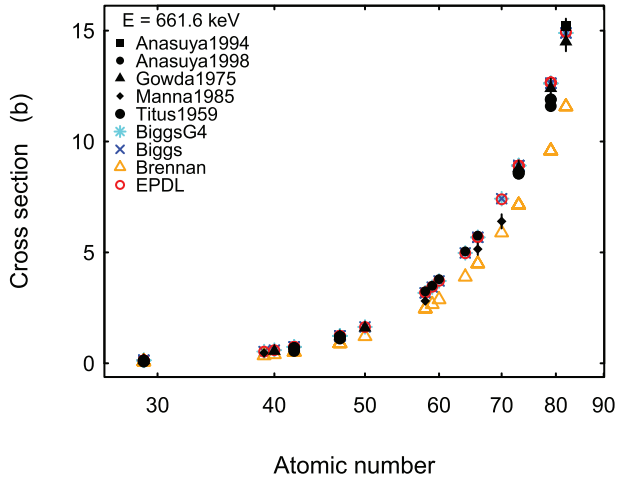
Main difficulty

Digging into the literature *(over almost a century…)* to extract experimental data, evaluate them for consistency, systematics etc.

Photoelectric effect

Total and shell (K, $L_{1,2,3}$) cross sections

- Biggs-Lighthill
- Brennan-Cowan
- Chantler
- Ebel
- Elam
- **EPDL97**
- Henke
- McMaster
- PHOTX
- RTAB
- Storm-Israel
- Veigele
- XCOM
- Sabbatucci-Salvat (2016)



Scofield's 1973 (EPDL) non-relativistic calculations **total** cross sections: state-of-the-art for Monte Carlo particle transport

Insufficient statistical evidence to prefer other calculations for **inner shell** cross sections

Lack of experimental data to assess **outer shell** cross sections

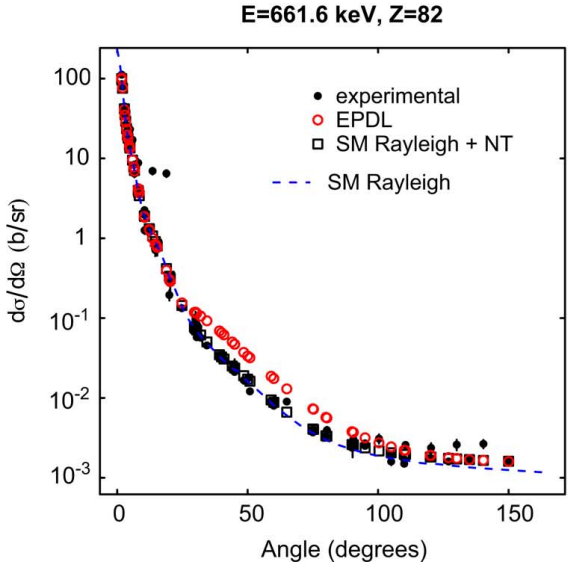
M. C. Han et al., "Validation of Cross Sections for Monte Carlo Simulation of the Photoelectric Effect", *IEEE Trans. Nucl. Sci.*, vol. 63, no. 2, pp. 1117–1146, 2016.

T. Basaglia et al., "Evolutions in photoelectric cross section calculations and their validation", *IEEE Trans. Nucl. Sci.,* vol. 67, no. 3, pp. 492-501, 2020.

ENDF data & GNDS **OK**

Photon elastic scattering

EPDL: Hubbell's non-relativistic form factors



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

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.

S-matrix calculations exhibit significantly better compatibility with experiment than EPDL approach based on form factor approximation

ENDF data & GNDS need extensions

(but do not drop current form factor data: diversity of requirements!)

Electron ionisation cross sections

Total cross section models

▲ Deutsch-Märk (DM)

■ Binary Encounter Bethe (BEB)

● EEDL

Need EEDL + other data

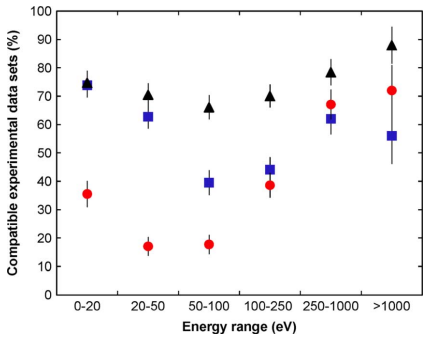


Fig. 6. Fraction of test cases in which cross sections calculated by the implemented models are compatible with experimental data at 0.05 significance level: BEB model (blue squares), DM model (black triangles) and EEDL (red circles). The fraction is calculated over the whole collection of data sets.

DM model reproduces total experimental cross sections better than EEDL below a few hundred eV

IEEE TRANSACTIONS ON NUCLEAR SCIENCE, VOL. 58, NO. 6, DECEMBER 2011 3219

Ionization Cross Sections for Low Energy Electron Transport

Hee Seo, Maria Grazia Pia, Paolo Saracco, and Chan Hyeong Kim

K shell cross section

EEDL OK

No significant difference in compatibility with experiment is observed between EEDL and recent calculations by Bote-Salvat in distorted wave approximation

PHYSICAL REVIEW A **77**, 042701 (2008)

Calculations of inner-shell ionization by electron impact with the distorted-wave and plane-wave Born approximations

David Bote* and Francesc Salvat†

Facultat de Física (ECM), Universitat de Barcelona, Diagonal 647, 08028 Barcelona, Spain

(Received 24 October 2007; published 1 April 2008)

$L_{1,2,3}$ cross sections

EEDL OK?

Univocal conclusions limited by scarcity of experimental data

IEEE TRANSACTIONS ON NUCLEAR SCIENCE, VOL. 65, NO. 8, AUGUST 2018 2279

Validation of Shell Ionization Cross Sections for Monte Carlo Electron Transport

Tullio Basaglia, Matteo Bonanomi, Federico Cattorini, Min Cheol Han, Gabriela Hoff, Chan Hyeong Kim, Sung Hun Kim, Matteo Marcoli, Maria Grazia Pia, and Paolo Saracco

Further major extensions

e.g stopping powers

Data for particles other than electrons/photons

Identify and document GNDS requirements

Verify if new format definitions are needed

How is requirements traceability implemented in GNDS project?

What are traceability items in GNDS project?

Resources are needed…

Conclusion

We wish nuclear and atomic data to progress together in their transition to GNDS

GNDS should effectively accommodate the requirements of atomic data

Atomic data libraries have been “orphan” for a long time… need time to catch up

(Support to our team’s research proposal to INFN would be helpful)

A **roadmap** for
electromagnetic data libraries and their GNDS encoding
+ adequate **resources** to do the wotk

Manifesto for Open Physics Data Libraries

IEEE Workshop (NSS-MIC), Manchester, 27 October 2019
Review paper in preparation for IEEE Trans. Nucl. Sci.