First assessment of new
Evaluated Data Libraries for Monte Carlo particle transport

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Foreword

Due to limited time allocation, there is room only to highlight a few results

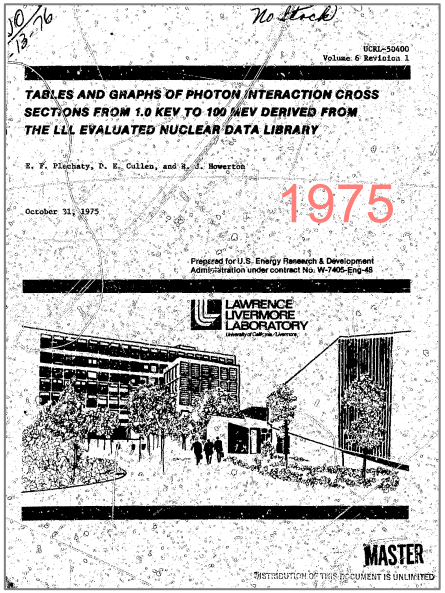
Evaluated data libraries

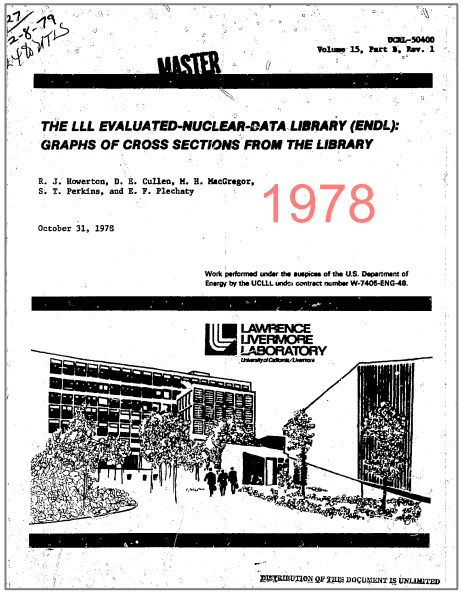
- Tabulations of physics quantities: cross sections, secondary particle spectra, nuclear and atomic parameters…
- Derived from the evaluation of the body of knowledge of **theoretical** computations, **experimental** measurements *or both*
- **Essential tool for Monte Carlo particle transport**
- BROND *(Russian Evaluated Neutron Data Library)*
- CENDL *(Chinese Evaluated Nuclear Data Library)*
- ENDF/B *(Evaluated Nuclear Data File)*
- JEFF *(Joint Evaluated Fission and Fusion File)*
- JENDL *(Japanese Evaluated Nuclear Data Library)*
- ENDF/B-VI: **1990**, ENDF/B-VII: **2006**, ENDF/B-VIII: **2018**

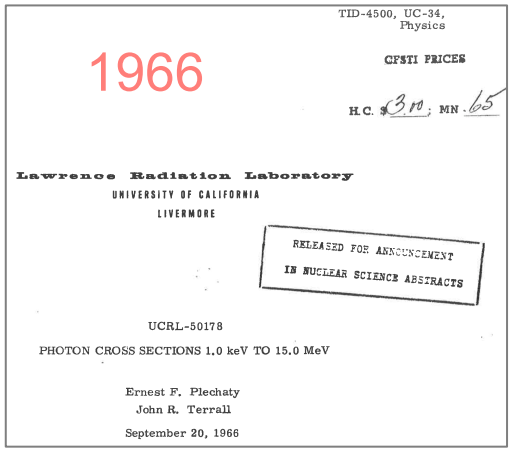
EGS, FLUKA, Geant4, MCNP, Penelope, PHITS…

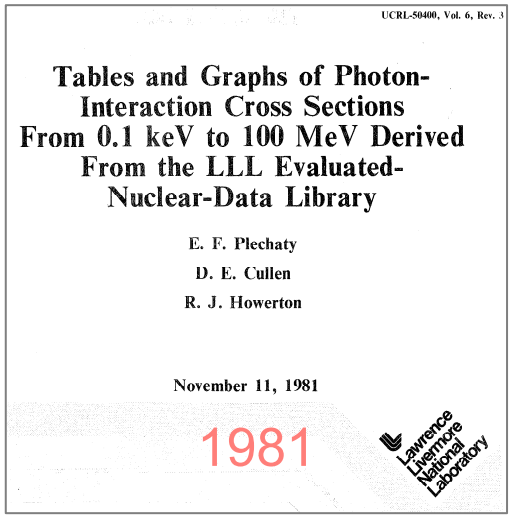
Evaluated Atomic Libraries

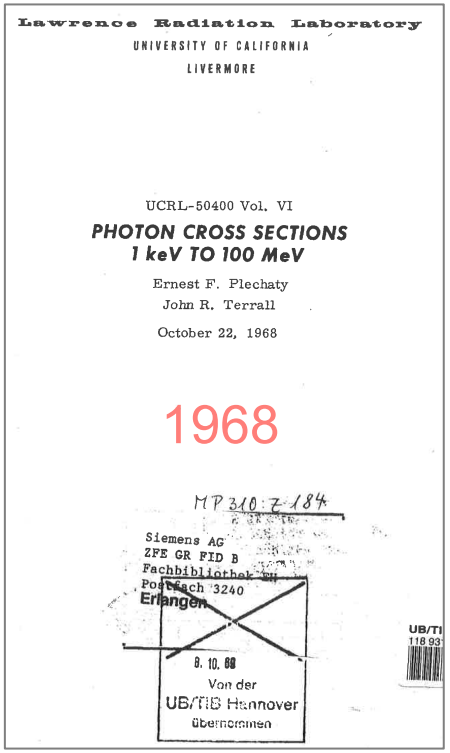
- **EADL** (atomic) **1991**
- **EEDL** (electron) **1991**
- **EPDL** (photon) **1997**

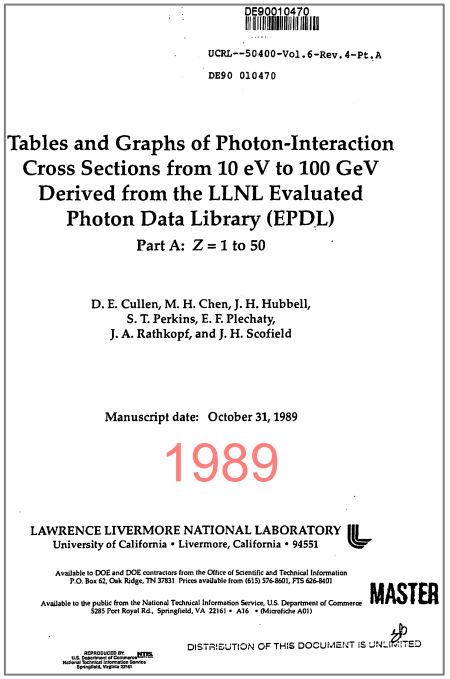












- **Originally released by LLL/LLNL**
- Released in **ENDF/B** since version **VI.8**
- Released by **IAEA** as **EPICS** since 2014

Formats:
ENDL
ENDF

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

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"

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

A Survey of Atomic Binding Energies for use in EPICS2017

IAEA-NDS-224
September 2017

by
Dermott E. Cullen

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

Contents lists available at ScienceDirect
Nuclear Instruments and Methods in Physics Research A
journal homepage: www.elsevier.com/locate/nima

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,**]

Validation

- of physics content (e.g. cross sections) w.r.t. measurements
- in comprehensive applications (e.g. energy deposition in a detector)
- Requirements for validity related to **use cases** *(IEEE Standard 1012 V&V)*
- **State of the art**: the best one can do, given the body of knowledge

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

References

- 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.
- L. Pandola et al., "Validation of the Geant4 simulation of Bremsstrahlung from thick targets below 3 MeV", *NIM B*, vol. 350, pp. 41–48, 2015.
- 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.

The world changes… 1991/1997 → 2018

- Kissel's S-matrix calculations of photon elastic scattering
- Electron ionisation cross sections *(Deutsch-Märk, Kim-Rudd, Bote-Salvat…)*
- Scofield's Hartree-Fock calculations of atomic parameters
- Effects of theoretical/experimental atomic binding energies
- Salvat's electron elastic scattering calculations
- Photoelectric cross sections, relativistic scattering functions etc.

Great expectations for new data libraries!

EPICS2017 Released in January 2018 by IAEA
Released in February 2018 in ENDF/B-VIII.0

D. E. Cullen, IAEA-NDS-0224 rev. 1, IAEA-NDS-0225 rev. 1, IAEA-NDS-0226, 2017

D. A. Brown et al., ENDF/B-VIII.0: The 8th Major Release of the Nuclear Reaction Data Library with CIELO-project Cross Sections, New Standards and Thermal Scattering Data, *Nucl. Data Sheets,* vol. 148, pp. 1-142, 2018

EPICS2014 "Modernized by reviewing recently published data and making changes" (D. E. Cullen, IAEA-NDS-218, rev.1, 2015)
No change observed, apart from fixing format conversion errors and scientific number notation

Content

Different content for different data formats

Not trivial to retrieve what contains what

Physics Data **EADL**	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

Physics Data **EPDL**	EPDL97		EPICS2014		EPICS2017	
	ENDL	ENDF-6	ENDL	ENDF-6	ENDL	ENDF-6
Total photon cross section	-	-	-	-	-	yes
Coherent scattering: integrated cross section	yes	yes	yes	yes	yes	yes
Coherent scattering: average energy of the scatterd photon	yes	-	yes	-	yes	-
Coherent scattering: form factor	yes	yes	yes	yes	yes	yes
Coherent scattering: imaginary anomalous scattering factor	yes	yes	yes	yes	yes	yes
Coherent scattering: real anomalous scattering factor	yes	yes	yes	yes	yes	yes
Incoherent scattering: integrated cross section	yes	yes	yes	yes	yes	yes
Incoherent scattering: scattering function	yes	yes	yes	yes	yes	yes
Incoherent scattering: average energy of the secondary particles	yes	-	yes	-	yes	-
Photoelectric: integrated cross section	yes	yes	yes	yes	yes	yes
Photoelectric: average energy to the residual atom	yes	-	yes	-	-	-
Photoelectric: average energy of secondary particles	yes	-	yes	-	-	-
Photoelectric: cross section by subshell	yes	yes	yes	yes	yes	yes
Photoelectric: average energy to the residual atom by subshell	yes	-	yes	-	yes	-
Photoelectric: average energy of secondary particles by subshell	yes	-	yes	-	yes	-
Pair production: integrated cross section	yes	yes	yes	yes	yes	yes
Pair production: average energy of secondary particles	yes	-	yes	-	yes	-
Triplet production: integrated cross section	yes	yes	yes	yes	yes	yes
Triplet production: average energy of secondary particles	yes	-	yes	-	yes	-
Pair and triplet production: integrated cross section	-	yes	-	yes	-	yes

Physics Data **EEDL**	EEDL91		EPICS2014		EPICS2017	
	ENDL	ENDF-6	ENDL	ENDF-6	ENDL	ENDF-6
Total electron cross section	-	-	-	-	-	yes
Large angle elastic scattering: integrated cross section	yes	yes	yes	yes	yes	yes
Large angle elastic scattering: average energy to the residual atom	yes	-	yes	-	yes	-
Large angle elastic scattering: average energy of the scattered electron	yes	-	yes	-	yes	-
Large angle elastic scattering: angular distributions	yes	yes	yes	yes	yes	yes
Elastic scattering: integrated cross section	yes	-	yes	-	yes	yes
Ionisation: integrated cross section	-	-	-	-	yes	yes
Ionisation cross section by subshell	yes	yes	yes	yes	yes	yes
Ionisation: average energy of secondary particles by subshell	yes	-	yes	-	yes	-
Ionisation: spectra of the recoil electron by subshell	yes	yes	yes	yes	yes	yes
Bremsstrahlung: integrated cross section	yes	yes	yes	yes	yes	yes
Bremsstrahlung: energy spectra of the secondary photon	yes	yes	yes	yes	yes	yes
Bremsstrahlung: average energy of the secondary photon	yes	yes	yes	yes	yes	yes
Bremsstrahlung: average energy of the secondary electron	yes	-	yes	-	yes	-
Excitation: integrated cross section	yes	yes	yes	yes	yes	yes
Excitation: average energy to the residual atom	yes	yes	yes	yes	yes	yes

Assessment

- What **has changed in EPICS2017** and **ENDF/B-VIII** w.r.t. the data libraries currently used by major Monte Carlo codes
  - **Consistency**
  - Computational **performance**
  - **Validity** w.r.t. experimental data: first results, *(in progress)*
- What **has not changed**
  - and has been previously (recently) identified as the state of the art
  - and does not reflect the state of the art
- How the data libraries are **released**
- How they are **maintained**

Reliability lies not only in the content, but also in the process!

- **Opportunities for improvement**

What's new in EPICS2017

Atomic binding energies

Propagated into other dependent physics quantities
(cross sections, transition energies etc.)

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

Previous: theoretical

New: empirical, Carlson + Williams

Electron kinetic energies

Previous: undocumented

New: undocumented

Coherent photon scattering
integrated cross sections

Changes also in the real and imaginary components of anomalous scattering factors

Previous: from numerically integrated calculations combining Thomson scattering, form factors and anomalous scattering factors

New: ?

EEDL excitation data

Different integrated cross sections and average energies for 17 elements

Roundoff effects?

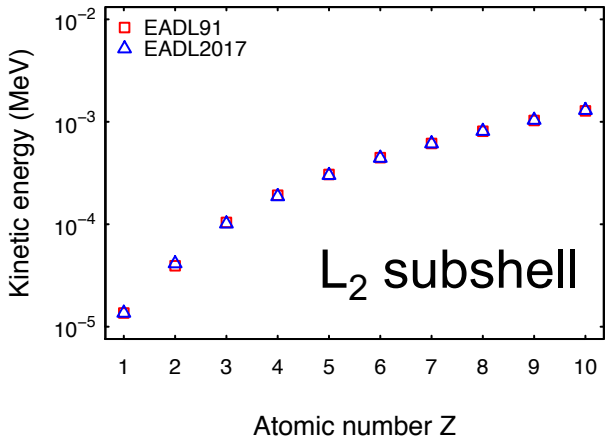
Elastic scattering, large angle scattering, Bremsstrahlung integrated cross sections

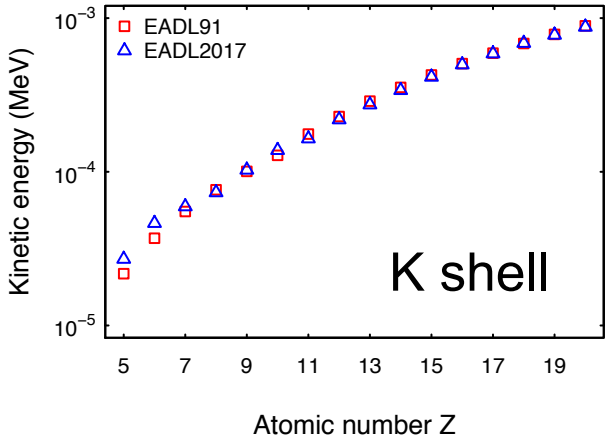
"Linearization"

Larger number of tabulated data to enable linear interpolation instead of logarithmic

Electron kinetic energies

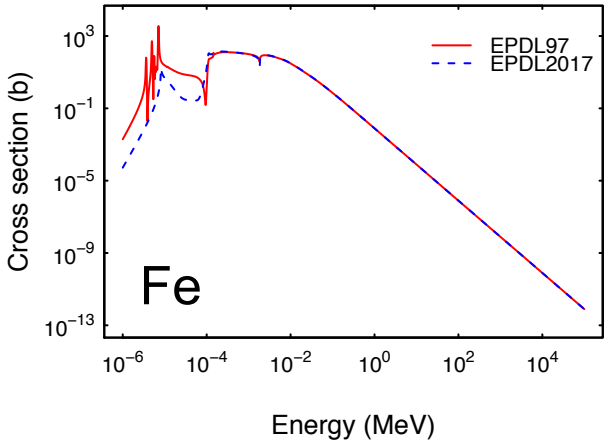
Experimental data for validation?

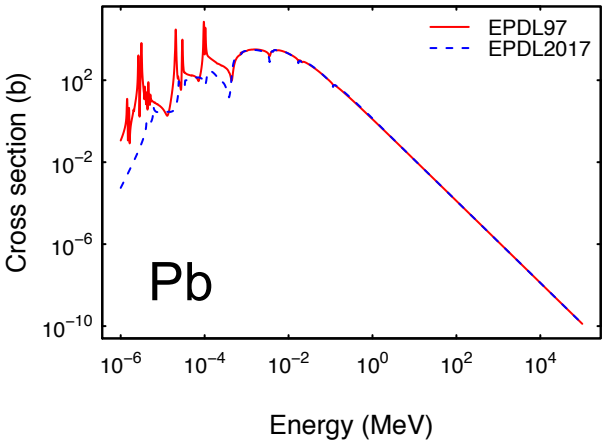




Differences appear larger for elements with low atomic numbers

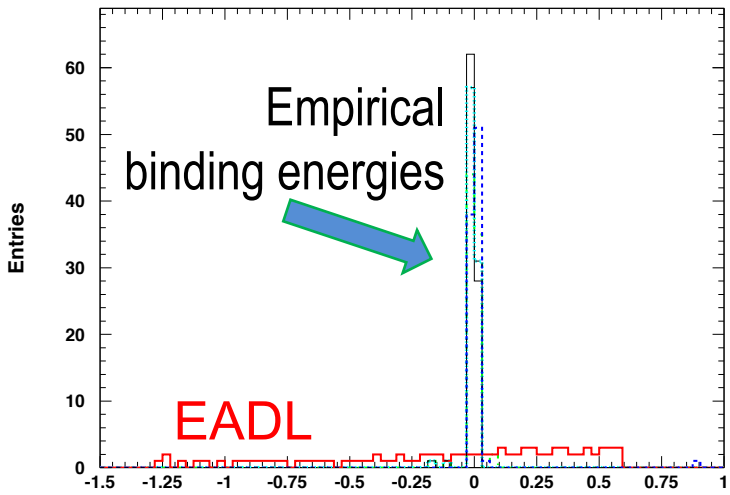
Coherent photon scattering integrated cross sections



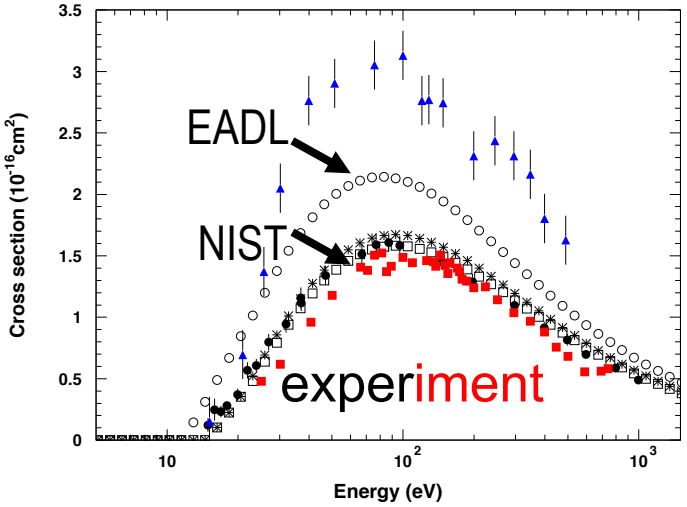


To the best of our knowledge, no experimental data available to validate the large changes at low energies

Atomic binding energies



Radiative transition energies, difference w.r.t. experiment



Electron ionisation cross sections calculated with EADL and NIST binding energies, w.r.t. experiment

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

In EPICS2017 and ENDF/B-VIII: **empirical** binding energies replaced previous theoretical values

…and their dependencies

e.g. relaxation data for carbon

6000.00000	11.9078164		0	0	4	0	60028533	1
1.00000000	0.0		0	0	54	8	60028533	2
288.000000	2.00000000	0.0	0.0	0.0	0.0		60028533	3
3.00000000	0.0	282.020000	5.61488D-4	0.0	0.0		60028533	4
4.00000000	0.0	282.030000	.001120600	0.0	0.0		60028533	5
2.00000000	2.00000000	255.890000	.413609000	0.0	0.0		60028533	6
2.00000000	3.00000000	264.460000	.136190000	0.0	0.0		60028533	7
2.00000000	4.00000000	264.470000	.271099000	0.0	0.0		60028533	8
3.00000000	3.00000000	273.030000	.004207480	0.0	0.0		60028533	9
3.00000000	4.00000000	273.040000	.110012000	0.0	0.0		60028533	10
4.00000000	4.00000000	273.050000	.063200800	0.0	0.0		60028533	11
2.00000000	0.0		0	0	6	0	60028533	12
16.5900000	2.00000000	0.0	0.0	0.0	0.0		60028533	13
3.00000000	0.0		0	0	6	0	60028533	14
11.2600000	.670000000	0.0	0.0	0.0	0.0		60028533	15
4.00000000	0.0		0	0	6	0	60028533	16
11.2600000	1.33000000	0.0	0.0	0.0	0.0		60028533	17

Radiative and non-radiative transition energies are **inconsistent** with atomic binding energies

non-conservation of energy!

Consistency issues

"Starting with EPICS2017 all the data has been **linearized** [...]. The result is libraries are roughly three (3) times as large, but it can be accurately interpolated using LIN- LIN interpolation…"

Not all the photon data in EPDL are tabulated with a larger number of energy points; in some cases fewer data than in EPDL97

Electron data have not been "linearized", but the documentation recommends linear interpolation

Different number of data points in ENDF/ENDL libraries, and in nominally identical libraries released by IAEA, ENDF/B and NNDC

Inconsistent (or intentionally modified?) **units** in form factors and scattering functions: **NOT DOCUMENTED**, liable to induce to errors in simulations

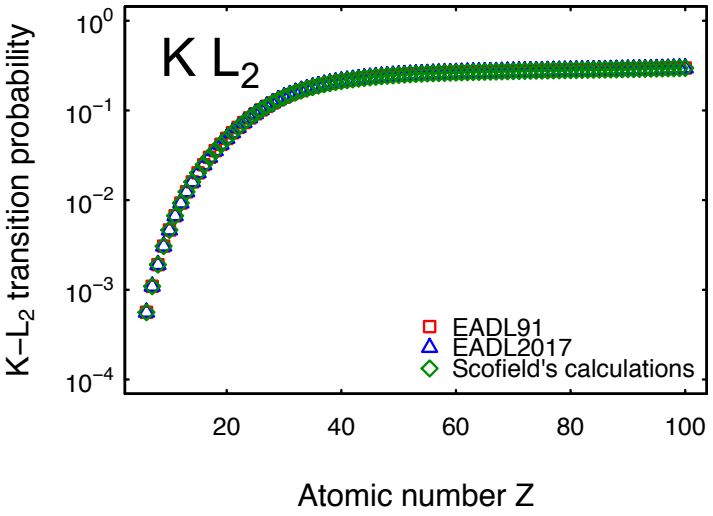
Non-monotonic primary e^- energies in secondary e^- spectra: interpolation problems

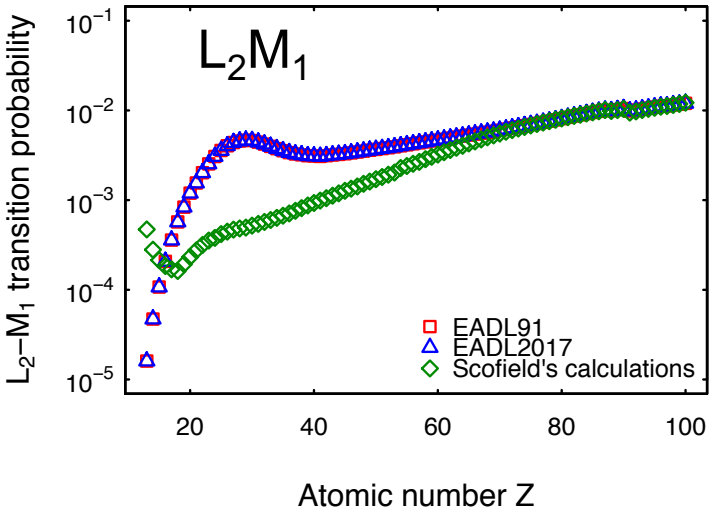
```
  6000  9 19  0.0         1712152 2  0.0          0.0          0.0
81 21 91  0.0          5.           0.0          0.0          0.0
 1.126000000D-05 2.525000000D-09 4.400440000D+07
 1.126000000D-05 2.525000000D-08 4.400440000D+07
 9.495000000D-06 2.525000000D-09 4.062760000D+06
 9.495000000D-06 2.525000000D-07 3.938040000D+06
```

also $E_{primary}$ < atomic binding E!

Physics issues

Radiative transition probabilities





EADL radiative transition probabilities derive from calculations of transition rates by Scofield

Discrepancies identified between EADL transition probabilities and Scofield's original calculations, which reproduce experimental data better than EADL

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.

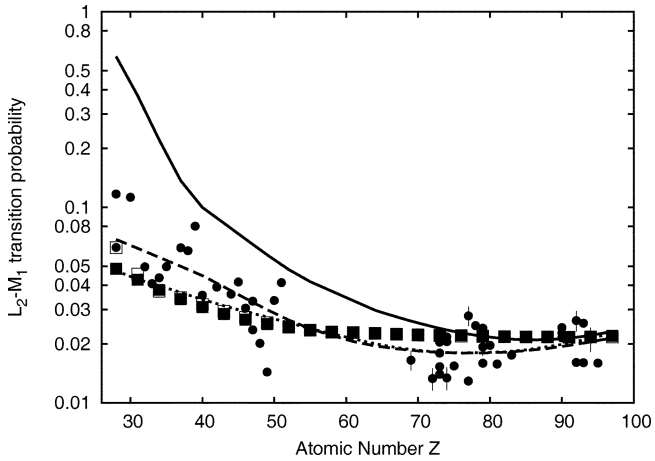


Fig. 12. L_2-M_1 transition probability versus Z: theoretical calculations based on the Hartree-Slater [2] (white squares) and the Hartree-Fock [3] (black squares) potentials, EADL [5] tabulations (solid line), experimental data (black circles), fit to them as in [13] (dashed line), and improved fit (dotted line).

The same discrepancies are still present in EPICS2017 and ENDF/B-VIII.0

Computational performance

MEMORY SIZE IN KB REQUIRED TO USE PHYSICS DATA OF ALL ELEMENTS

Physics data **Memory**	Original libraries	ENDF/B-VIII EPICS2017	Ratio
Bremsstrahlung cross section	368	368	1
Elastic scattering cross section	472	472	1
Large angle elastic scattering cross section	472	472	1
Ionisation cross section by subshell	1924	1924	1
Excitation cross section	1152	1152	1
Coherent scattering cross section	4528	1868	0.4
Coherent scattering form factor	708	4620	6.5
Incoherent scattering cross section	508	1692	3.3
Incoherent scattering scattering function	724	1836	2.5
Photoelectric cross section	4480	32620	7.3
Photoelectric cross section by subshell	7536	45976	6.1
Pair production cross section	496	1356	2.7
Triplet production cross section	436	920	2.1

COMPUTATIONAL TIME IN SECONDS TO CALCULATE INTEGRATED CROSS SECTIONS WITH DIFFERENT INTERPOLATION METHODS

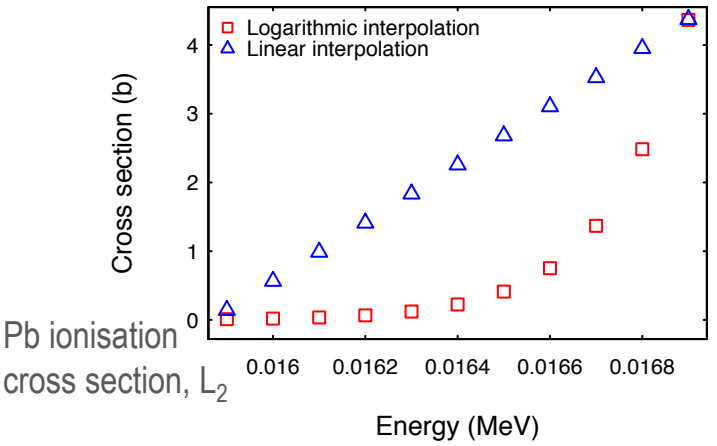
Physics process **CPU**	Original Libraries Logarithmic	EPICS2017 Linear
Bremsstrahlung	3.88 ± 0.01	0.63 ± 0.01
Elastic scattering	3.90 ± 0.01	0.79 ± 0.01
Large angle elastic scattering	3.92 ± 0.01	0.79 ± 0.01
Excitation	4.21 ± 0.01	1.06 ± 0.01
Coherent scattering	4.32 ± 0.02	1.21 ± 0.01
Incoherent scattering	3.93 ± 0.01	1.28 ± 0.01
Photoelectric	4.67 ± 0.01	3.68 ± 0.01
Pair production	2.36 ± 0.01	0.85 ± 0.01
Triplet production	2.25 ± 0.01	0.81 ± 0.01

Results with a trivial data management software
Can do much better with smarter algorithms

"Linearized" data libraries:

tradeoff between memory and CPU needs

Related to the characteristics of each experimental scenario



Pb ionisation cross section, L_2

Beware of **precision of interpolation** of electron data: linear interpolation recommended in EEDL documentation, but same number of points as in EEDL1991!

ISO/IEC/IEEE 12207
IEEE Standard 828

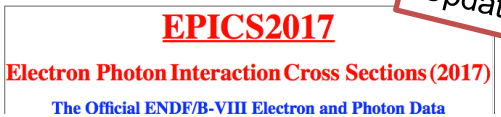
Reproducibility issues

- Inconsistencies between the **same data** released in **ENDF** and **ENDL** format
- Inconsistencies between the **same data** in the **same format** released in **different systems**, e.g. EPICS2017 and ENDF/B-VIII.0
- Differences between the data released by **IAEA** and by **NNDC** as EPICS2017
- **Different data** released by IAEA under the **same identifier** of EPICS2017
  - e.g. photoelectric cross sections modified in February, all identified as EPICS2017
  - Same issue again with transition energies modified in April 2018

Example: Carbon

(screenshots on 18/6/2018)

Updated!



(http://www.nndc.bnl.gov/endf/epics/)

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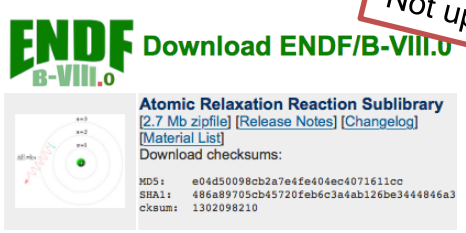
288.000000	2.00000000	0.0	0.0
3.00000000	0.0	276.740000	5.61488D-4
4.00000000	0.0	276.740000	.001120600
2.00000000	2.00000000	254.820000	.413609000
2.00000000	3.00000000	260.150000	.136190000
2.00000000	4.00000000	260.150000	.271099000
3.00000000	3.00000000	265.480000	.004207480
3.00000000	4.00000000	265.480000	.110012000
4.00000000	4.00000000	265.480000	.063200800
2.00000000	0.0	0	0
16.5900000	2.00000000	0.0	0.0
3.00000000	0.0	0	0
11.2600000	.670000000	0.0	0.0
4.00000000	0.0	0	0
11.2600000	1.33000000	0.0	0.0

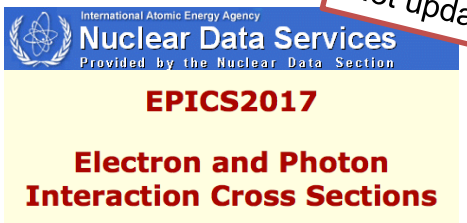
Not updated!



(http://www.nndc.bnl.gov/endf/b8.0)

6000.00000	11.9078164	0	0
1.00000000	0.0	0	0
288.000000	2.00000000	0.0	0.0
3.00000000	0.0	282.020000	5.61488D-4
4.00000000	0.0	282.030000	.001120600
2.00000000	2.00000000	255.890000	.413609000
2.00000000	3.00000000	264.460000	.136190000
2.00000000	4.00000000	264.470000	.271099000
3.00000000	3.00000000	273.030000	.004207480
3.00000000	4.00000000	273.040000	.110012000
4.00000000	4.00000000	273.050000	.063200800
2.00000000	0.0	0	0
16.5900000	2.00000000	0.0	0.0
3.00000000	0.0	0	0
11.2600000	.670000000	0.0	0.0
4.00000000	0.0	0	0
11.2600000	1.33000000	0.0	0.0

Not updated!



(https://www-nds.iaea.org/epics/)

6000.00000	11.9078164	0	0
1.00000000	0.0	0	0
288.000000	2.00000000	0.0	0.0
3.00000000	0.0	282.020000	5.61488D-4
4.00000000	0.0	282.030000	.001120600
2.00000000	2.00000000	255.890000	.413609000
2.00000000	3.00000000	264.460000	.136190000
2.00000000	4.00000000	264.470000	.271099000
3.00000000	3.00000000	273.030000	.004207480
3.00000000	4.00000000	273.040000	.110012000
4.00000000	4.00000000	273.050000	.063200800
2.00000000	0.0	0	0
16.5900000	2.00000000	0.0	0.0
3.00000000	0.0	0	0
11.2600000	.670000000	0.0	0.0
4.00000000	0.0	0	0
11.2600000	1.33000000	0.0	0.0

First validation test

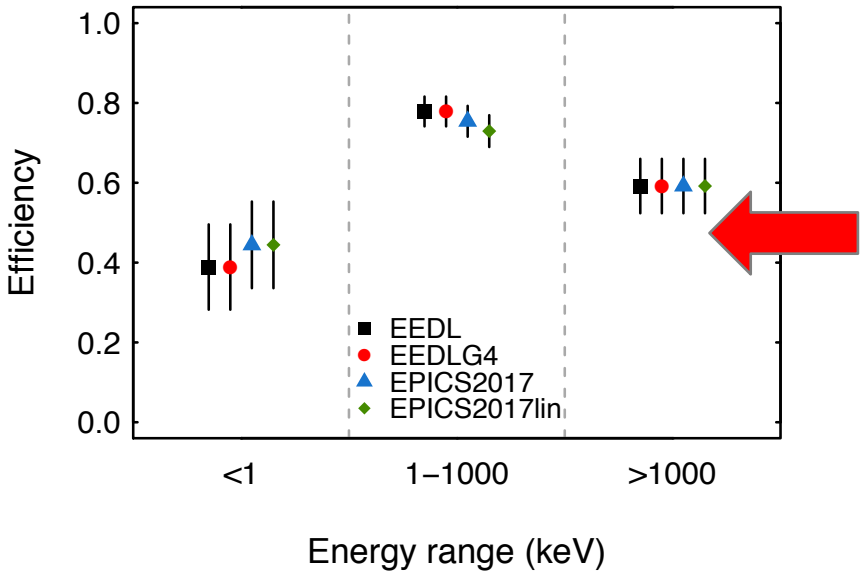
Electron ionisation cross sections

~ 2800 K shell cross section measurements

Goodness-of-fit tests
- χ^2
- Anderson-Darling
- Cramer-von Mises
- Kolmogorov-Smirnov

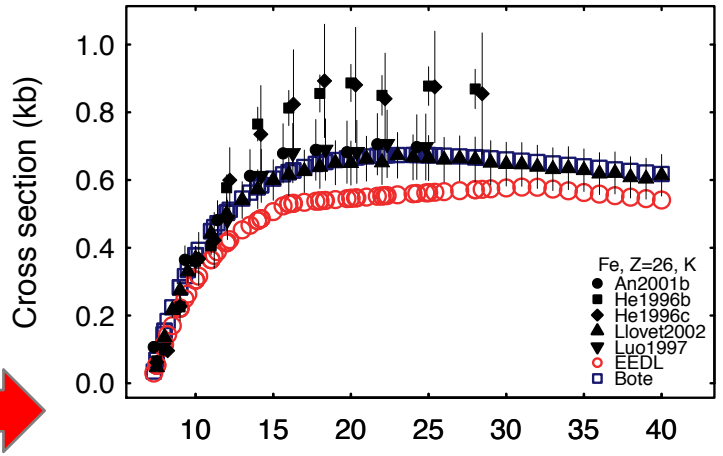
efficiency = fraction of test cases where H0 is not rejected

0.01 significance



Slightly different results with EPICS2017 w.r.t. EEDL91, but the difference in compatibility with experiment is **not statistically significant**

…but interpolation issues due to the coarse granularity of tabulations!



Conclusion

First assessment of long-awaited new versions of widely used Evaluated Atomic Data Libraries

Promising move from theoretical atomic binding energies to empirical ones

Other physics improvements identified by validation tests not yet included

Ample room for improvement in quality assurance

Critical: version control

Responsibility of the scientific community

M. C. Han et al., "First Assessment of ENDF/B-VIII and EPICS Atomic Data Libraries", *IEEE Trans. Nucl. Sci.*, https://doi.org/10.1109/TNS.2018.2849328

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Min Cheol Han