General overview of ENDF atomic data libraries

D. A. Brown

National Nuclear Data Center

Brookhaven National Laboratory

BROOKHAVEN NATIONAL LABORATORY

U.S. DEPARTMENT OF ENERGY

There are many users of ENDF/B-VIII.0 electro-, photo-atomic data

- **GEANT4**
  (POC for e^-, γ transport:
  M. G. Pia, INFN Genova)
- **PHITS**
  (https://phits.jaea.go.jp)
  (POC: T. Furuta, JAEA)
- **FLUKA** (fluka.org)
- **MCNP**
- **PENELOPE**
  (POC: F. Salvat, U. Barcelona)
  - Integrated into **penORNL**
- **EGS**, obsolete but forked into
  - **EGSnrc** (https://nrc-cnrc.github.io/EGSnrc)
  - **EGS5** integrated into PHITS
- **ITS** (POC: B. Franke, SNL)
- **SCEPTRE**
  (POC: C. Drumm, SNL)
- **CEPXS** (SNL)
- Method development codes:
  - **FRENSIE** (U. Wisconsin),
  - **P++** (RPI)

And this doesn't even include XRF users!

ENDF atomic sublibraries

The ENDF photo-atomic sublibrary

- **Coherent scattering,**
  - ***integrated cross section (b),***
  - ***form factor,***
  - ***real and imaginary anomalous scattering factors,***
  - average energy of the scattered photon (MeV),
- **Incoherent scattering**
  - ***integrated cross section (b),***
  - ***scattering function,***
  - average energy of the scattered photon and recoil electron (MeV).
- **Total photoelectric reaction**
  - ***integrated cross section (b),***
  - average energy to the residual atom, i.e., local deposition (MeV),
  - average energy of the secondary photons and electrons (MeV).
- **Photoelectric reaction, by subshell**
  - ***integrated cross section (b),***
  - average energy to the residual atom, i.e., local deposition (MeV),
  - average energy of the secondary photons and electrons (MeV) .
- **Pair production reaction**
  - ***integrated cross section (b),***
  - average energy of the secondary electron and positron (MeV) .
- **Triplet production reaction**
  - ***integrated cross section (b),***
  - average energy of the secondary electron and positron (MeV) .

green == FUDGE can plot

The ENDF electro-atomic sublibrary

- **Elastic transport,**
  - ***transport cross section, σ_{el} (1-E<cosθ>) (b)***
- **Large angle elastic scattering (over cosθ = -l. to 0.999999)**
  - ***integrated LACS cross section (b),***
  - average energy of the scattered electron (MeV),
  - average energy to the residual atom, i.e., local deposition (MeV),
  - angular distribution of the scattered electron.
- **Elastic scattering**
  - ***integrated scattering cross section (b),***
- **Ionization, by subshell**
  - ***integrated cross section (b),***
  - average energy to the scattered and recoil electron (MeV)
  - spectra of the recoil electron (MeV^{-1}).
- **Bremstrahlung**
  - ***integrated cross section (b),***
  - average energy of the secondary electron and photon (MeV) ,
  - spectra of the secondary photon (MeV^{-1}).
- **Excitation**
  - ***integrated cross section (b),***
  - average energy to the residual atom, i.e., local deposition (MeV).

green == FUDGE can plot

The ENDF atomic relaxation sublibrary

- **Subshell data**
  - number of electrons,
  - binding and kinetic energy (MeV),
  - average radius (cm),
  - radiative and nonradiative level widths (MeV),
  - average number of released electrons and x-rays,
  - average energy of released electrons and x-rays (MeV),
  - average energy to the residual atom, i.e., local deposition (MeV).
- **Transition probability data**
  - radiation transition probabilities,
  - nonradiative transition probabilities.

What parts of this data can we test? How can we test this data?

History of ENDF atomic sublibraries

Designation	Date	ENDF/B	Comments
DLC-7/HPICE	Sep. 1969	n/a	Initial release
DLC-7C/HPICE	Jan. 1970	ENDF/B-II	Named ENDF/B-II photon interaction library
DLC-7D/HPICE	Apr. 1971	ENDF/B-III	Pair production increased by 3-5%; incoherent scat. corrected 0.8 MeV for Z=31-34
DLC-7E/HPICE	July 1975	ENDF/B-IV	File 27 data added & replaced file 23 cross sections
DLC-7F/HPICE	Oct. 1975	ENDF/B-IV	Update previous data with new 1973 Fundamental Constants
DLC-99/HUGO	Dec. 1983	ENDF/B-V	Updated with new National Bureau of Standards data; new ENDF/B-V format
EPDL89	1989	ENDF/B-VI	S. Perkins & Red Cullen's EPDL, see UCRL-50400 Vol. 6 Rev. 4 (1989); photons from 10 eV — 100 GeV
EEDL91	1991	ENDF/B-VI	UCRL-50400 Vol. 31 (1991) — EEDL
EPDL97	1997	ENDF/B-VI	photons extended down to 1 eV, add photoionization to compute anomalous scattering factors, photo-excitation data
EADL	2001	ENDF/B-VI	UCRL-50400 Vol. 30 (2001) — EADL
EPICS2014	2014	n/a	
EPICS2017	2017*	ENDF/B-VIII.0	

see Roussin, et al. ENDF-335 (1983)

EPICS2014 consists of 4 libraries

- ***The Evaluated Electron Data Library (EEDL)***,
  to describe the interaction of electrons with matter.
- ***The Evaluated Photon Data Library (EPDL),***
  to describe the interaction of photons with matter.
- ***The Evaluated Atomic Data Library (EADL),***
  to describe the emission of electrons and photons back to neutrality following an ionizing event, caused by either electron or photon interactions
- ***The Evaluated Excitation Data Library (EXDL),***
  to describe the excitation of atoms due to photon interaction

EPICS2014 consists of 4 libraries

- ***The Evaluated Electron Data Library (EEDL)***,
  to describe the interaction of electrons with matter.
- ***The Evaluated Photon Data Library (EPDL),***
  to describe the interaction of photons with matter.
- ***The Evaluated Atomic Data Library (EADL),***
  to describe the emission of electrons and photons back to neutrality following an ionizing event, caused by either electron or photon interactions
- ***The Evaluated Excitation Data Library (EXDL),***
  to describe the excitation of atoms due to photon interaction

In ENDF & ENDL formats

EPICS2014 consists of 4 libraries

- ***The Evaluated Electron Data Library (EEDL)***,
  to describe the interaction of electrons with matter.
- ***The Evaluated Photon Data Library (EPDL),***
  to describe the interaction of photons with matter.
- ***The Evaluated Atomic Data Library (EADL),***
  to des… …k to
  neutra…
  electron or photon interactions

In ENDL format only

- ***The Evaluated Excitation Data Library (EXDL),***
  to describe the excitation of atoms due to photon interaction

EPICS2014

- **Major changes:**
  - Corrected incorrectly translated electron data (MF/MT=26/527, <E> from Bremstrahlung)
  - Increase file precision with ENDF2C
  - “Changes where I felt they were necessary”
- **Major change not made:**
  - Revising transition energies to match results of Deslattes, et al., “X-ray transition energies: a new approach to a comprehensive evaluation”, Rev. Mod. Phys. **75**, 35-99 (2003).
- **Update seems minor, but important to upgrade all sub libraries as a set to maintain internal consistency**

The process broke down with EPICS2017, used in ENDF/B-VIII.0

Maria Grazia Pia (INFN) presented a thorough and critical review of the new atomic transport data in ENDF/B-VIII.0

- GEANT4 Physics Developments and Validation page (https://www.ge.infn.it/geant4/index.html)
- This talk's content from https://www.ge.infn.it/geant4/talks/rpsd2018/datalib.pdf and posted in indico
- IEEE Trans. Nucl. Sci. (https://doi.org/10.1109/TNS.2018.2849328).
- Other papers concerning EADL/EEDL/EPDL validation published by her research group are listed in https://www.ge.infn.it/geant4/papers/index.html


Maria Grazia Pia

She couldn't make it to CSEWG, but is very interested in collaborating with us

Formatting problems with EPICS

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

Version control issues with EPICS

Example: Carbon

(screenshots on 18/6/2018)

Updated!

EPICS2017

Electron Photon Interaction Cross Sections (2017)

The Official ENDF/B-VIII Electron and Photon Data

(http://www.nndc.bnl.gov/endf/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         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!

ENDF B-VIII.0 Download ENDF/B-VIII.0

Atomic Relaxation Reaction Sublibrary

[2.7 Mb zipfile] [Release Notes] [Changelog] [Material List]

Download checksums:

MD5: e04d50098cb2a7e4fe404ec4071611cc

SHA1: 486a89705cb45720feb6c3a4ab126be3444846a3

cksum: 1302098210

(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!

International Atomic Energy Agency

Nuclear Data Services

Provided by the Nuclear Data Section

EPICS2017

Electron and Photon Interaction Cross Sections

(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
```


- Red sent final version in April, well after ENDF/B-VIII.0 released.
- Final version fixes consistency problems with binding energies

- Not reflected in ENDF/B-VIII.0 release tarballs nor IAEA page, only EPICS page and ENDF/B-VIII.0 Errata page
- We look like idiots and I'm p*ssed
- More importantly, users are VERY confused

First validation test

Electron ionisation cross sections

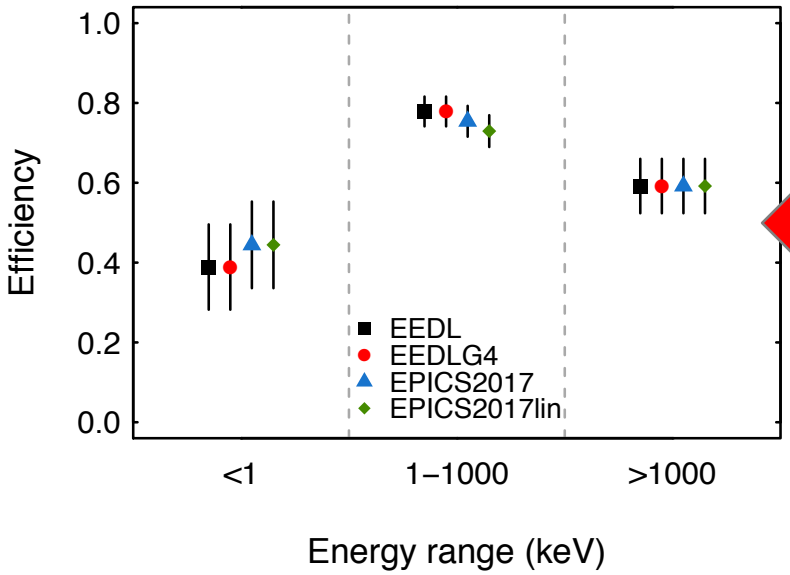
~ 2800 K shell cross section measurements

Goodness-of-fit tests

- χ^2
- Anderson-Darling
- Cramer-von Mises
- Kolmogorov-Smirnov

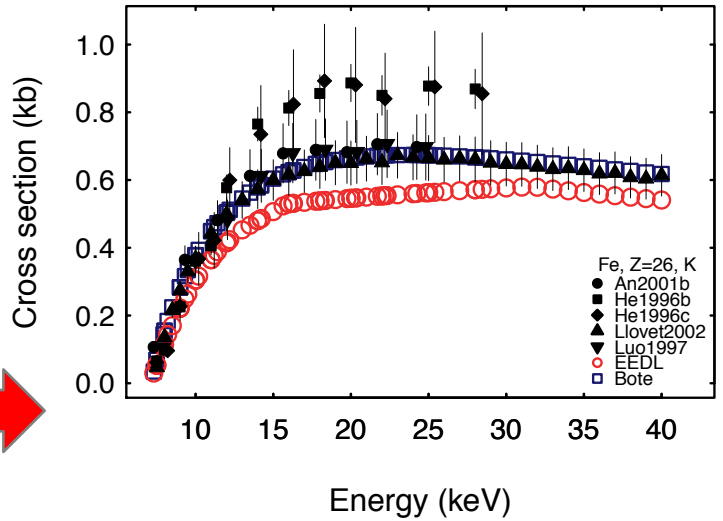
0.01 significance level

efficiency = fraction of test cases where H0 is not rejected



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

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



Summary of shortcomings

- **Documentation**:
  - Unclear what was improved in this release (Red's documentation "incomplete")
  - What is documented is not what is in files
  - ENDF documentation that clarified formats used by author only generally available after release
- **Version control**:
  - Library content is format dependent (ENDL vs. ENDF/GNDS)
  - Version screwups due to blowing past deadline
- **Verification rushed:**
  - Binding energy error could have been caught with time (EADL unchecked), eliminating post-release errata
- **Validation issues:**
  - Precision choices made by author impact validation
  - No apparent validation done by author and we had no contacts that could perform validation
  - Validation by Grazia Pia's groups found issues

In lieu of the many users of these libraries, we need help so we don't repeat this mess-up

Status of CSEWG collaborations support of ENDF atomic data

- **CSEWG owns ENDF**
  - No one currently in CSEWG knows much about atomic data
  - (you all are welcome to join CSEWG, just show up at nuclear data week!)
  - Current POC is LLNL retiree (Red Cullen)
  - Outside of Red, very little coordination between data developers and users
- **Major gaps in manpower**
  - “No evaluators”
  - Very few of us understand ENDF (or GNDS) format for atomic data
  - Processing not well understood anymore
  - Validation capabilities standing up (again) at SNL, LANL, very strong at INFN
  - Large user base disconnected from rest of process
- **Should we have a discussion about expanding the scope of ENDF atomic data?**