General overview of ENDF atomic data libraries

D. A. Brown
National Nuclear Data Center
Brookhaven National Laboratory
There are many users of ENDF/B-VIII.0 electro-, photo-atomic data

- **GEANT4**
  (POC for e\(^-\), \(\gamma\) transport:
  M. G. Pia, INFN Genova)
- **PHITS**
  ([https://phits.jaea.go.jp](https://phits.jaea.go.jp))
  (POC: T. Furuta, JAEA)
- **FLUKA** ([fluka.org](http://fluka.org))
- **MCNP**
- **PENELOPE**
  (POC: F. Salvat, U. Barcelona)
  * Integrated into **penORNL**
- **EGS**, obsolete but forked into
  - **EGSnrc** ([https://nrc-cnrc.github.io/EGSnrc](https://nrc-cnrc.github.io/EGSnrc))
  - **EGS5** integrated into PHITS
- **ITS** (POC: B. Franke, SNL)
- **SCEPTRE**
  (POC: C. Drumm, SNL)
- **CEPX5** (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).
The ENDF electro-atomic sublibrary

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

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
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In ENDF & ENDL formats
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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:

• 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](https://www.ge.infn.it/geant4/index.html))

• This talk’s content from [https://www.ge.infn.it/geant4/talks/rpsd2018/datalib.pdf](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](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](https://www.ge.infn.it/geant4/papers/index.html)

She couldn’t make it to CSEWG, but is very interested in collaborating with us
## Formatting problems with EPICS

### Content

<table>
<thead>
<tr>
<th>Physics Data</th>
<th>EADL</th>
<th>EPDL</th>
<th>EEDL</th>
</tr>
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<tbody>
<tr>
<td>Number of electrons</td>
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<td>yes</td>
</tr>
<tr>
<td>Binding energy</td>
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<td>yes</td>
</tr>
<tr>
<td>Kinetic energy</td>
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</tr>
<tr>
<td>Average radius</td>
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<td>yes</td>
<td>yes</td>
</tr>
<tr>
<td>Radiative level width</td>
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<tr>
<td>Non-radiative level width</td>
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<tr>
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<td>yes</td>
</tr>
<tr>
<td>Average energy of particles per initial vacancy</td>
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<td>yes</td>
<td>yes</td>
</tr>
<tr>
<td>Average number of particles per initial vacancy</td>
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<td>yes</td>
</tr>
<tr>
<td>Non-radiative transition probability and emitted particle energy</td>
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<td>yes</td>
<td>yes</td>
</tr>
<tr>
<td>Ionisation cross section by subshell</td>
<td>yes</td>
<td>yes</td>
<td>yes</td>
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<tr>
<td>Ionisation spectra of the recoil electron by subshell</td>
<td>yes</td>
<td>yes</td>
<td>yes</td>
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<tr>
<td>Ionisation: average energy of secondary particles by subshell</td>
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<td>Ionisation: integrated cross section</td>
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<tr>
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<tr>
<td>Photoelectric: average energy of secondary particles</td>
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<tr>
<td>Photoelectric: cross section by subshell</td>
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<td>Photoelectric: average energy to the residual atom by subshell</td>
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<td>Photoelectric: average energy of secondary particles by subshell</td>
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<td>yes</td>
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<tr>
<td>Elastic scattering: integrated cross section</td>
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<td>-</td>
<td>-</td>
</tr>
<tr>
<td>Total electron cross section</td>
<td>-</td>
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<td>Large angle elastic scattering: integrated cross section</td>
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<td>Large angle elastic scattering: average energy to the residual atom</td>
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<tr>
<td>Large angle elastic scattering: average energy of the scattered electron</td>
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<td>yes</td>
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<td>Elastic scattering: angular distributions</td>
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<td>Ionsation: integrated cross section</td>
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<td>yes</td>
<td>yes</td>
</tr>
<tr>
<td>Ionsation cross section by subshell</td>
<td>yes</td>
<td>yes</td>
<td>yes</td>
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<tr>
<td>Ionsation: average energy of secondary particles by subshell</td>
<td>yes</td>
<td>yes</td>
<td>yes</td>
</tr>
<tr>
<td>Ionsation: spectra of the recoil electron by subshell</td>
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<td>yes</td>
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<tr>
<td>Bremsstrahlung: integrated cross section</td>
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<tr>
<td>Bremsstrahlung: energy spectra of the secondary photon</td>
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<tr>
<td>Bremsstrahlung: average energy of the secondary photon</td>
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<tr>
<td>Bremsstrahlung: average energy of the secondary electron</td>
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<td>yes</td>
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<td>Excitation: integrated cross section</td>
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<td>yes</td>
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</tr>
<tr>
<td>Excitation: average energy to the residual atom</td>
<td>yes</td>
<td>yes</td>
<td>yes</td>
</tr>
</tbody>
</table>

### Different content for different data formats

Not trivial to retrieve what contains what
Version control issues with EPICS

**Example: Carbon**

(screeshots on 18/6/2018)

Not updated!

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

efficiency = fraction of test cases where H0 is not rejected

Goodness-of-fit tests
- $\chi^2$
- Anderson-Darling
- Cramer-von Mises
- Kolmogorov-Smirnov

0.01 significance level

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!

Maria Grazia Pia, INFN Genova
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?