Atomic data in the ENDF library

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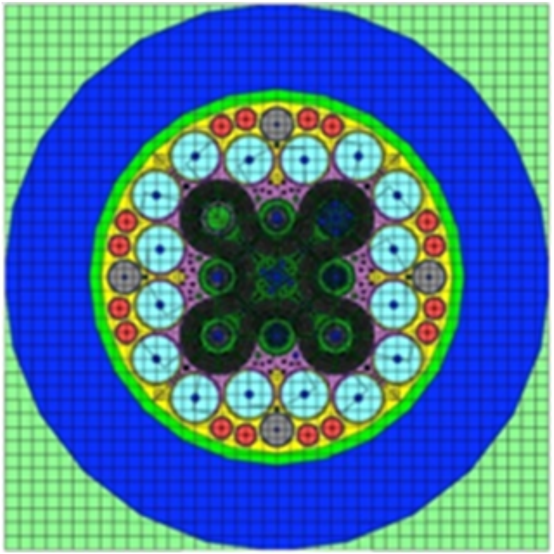
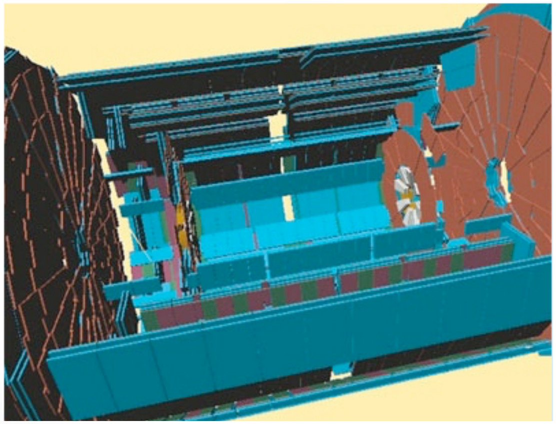
Atomic & nuclear data underpin many different codes

- **MCNP6, SCALE, & GEANT4 particle transport codes**
    - used for simulating nuclear energy generation
    - shielding and health physics calculations
- **ORIGEN & CINDER for isotope burn-up**
    - nuclear waste management
    - radiochemical applications
- **All have modules that use ENDF/ENSDF data**
- **Codes switch between models and data tables based on:**
    - speed
    - fidelity to physics
- **Other code systems also use covariance data in uncertainty quantification (e.g. SCALE's TSUNAMI)**



SCALE model of INL Advanced Test Reactor



ATLAS detector muon system, simulated in GEANT4

The ENDF Library is the US's most widely used nuclear data library

ENDF B-VIII.0

ENDF/B-VIII.0 was released on 2 Feb. 2018

Library and evaluations detailed in Nuclear Data Sheets vol. 148 (2018)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ELSEVIER

Nuclear Data Sheets

A Journal Devoted to Compilations and Evaluations of Experimental and Theoretical Results in Nuclear Physics

E. A. McCutchan, Editor
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www.nndc.bnl.gov

Special Issue on Nuclear Reaction Data

Special Issue Editor: Pavel Obložinský
Special Issue Assistant Editor: Boris Pritychenko

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Happy 50th Anniversary!*

* ENDF/B-I was released in June 1968

The Cross Section Evaluation Working Group

- **Formed 1966 at behest of US's Atomic Energy Commission**
  - Oldest scientific technical collaboration at BNL, maybe US?
  - Predates DOE by ~10 years
- **Main product is ENDF/B library**
- **Library users are also library producers**
  - If you see something in the library, at some point a sponsor somewhere wanted it
- **Large & diverse user/producer base**
  - Each user/producer contributes differently to greater good (experiments vs. evaluations vs. validation)
  - My needs don't equal yours, but if we work together, we all benefit
- **Chaired by NNDC at BNL**

TRIUMF

Argonne NATIONAL LABORATORY

Canadian Nuclear Laboratories

Laboratoires Nucléaires Canadiens

CSEWG Cross Section Evaluation Working Group

Rensselaer

Berkeley Lab

Lawrence Livermore National Laboratory

Sandia National Laboratories

Los Alamos NATIONAL LABORATORY EST. 1943

Oak Ridge National Laboratory

U.S. DEPARTMENT OF ENERGY

BROOKHAVEN NATIONAL LABORATORY

NAVAL NUCLEAR LABORATORY

NIST

NC STATE UNIVERSITY

CNEA

BROOKHAVEN NATIONAL LABORATORY

CSEWG is not limited to the Americas

CSEWG
Cross Section Evaluation Working Group

AWE
NRG
European Commission
Joint Research Centre

The ENDF Library contains 3 sub libraries with an atomic focus

- **Collisional Data:**
  - Photo-atomic Sublibrary
  - Electro-atomic Sublibrary

For use in electron and photon transport through neutral material in the energy range ~10 eV - 1 GeV (shielding, medical imaging, detector development, …)

- **Spectroscopic Data:**
  - Atomic-relaxation Sublibrary

Data to describe emissions following knock-out of an e- (medical imaging, decay heat from spent fuel, XRF, …)

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) .

Anything needed to transport photons

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).

Anything needed to transport electrons

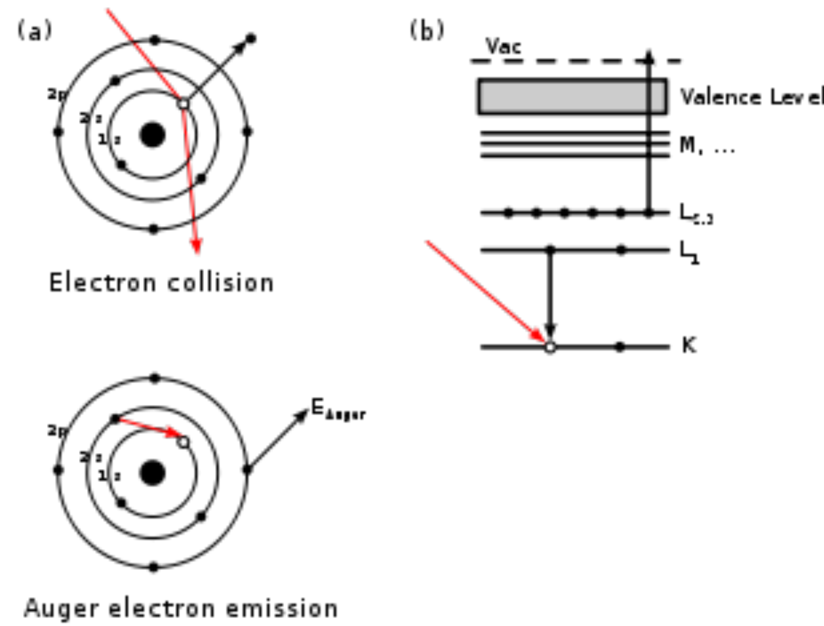
ENDF electro- & photo-atomic data are used in several well known transport codes

- **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)

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.



Used:
- To simulate e^- & γ emissions after a nuclear decay
- Source for X-ray lines in several XRF analysis codes

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)

For most of ENDF's history, atomic data was side-project of D.E. (Red) Cullen

- **Maintained through a collaboration with NIST**
- **Data needed by LLNL programs**
  - Primary format was LLNL's internal format: ENDL
  - Porting to ENDF happened later
- **Red retired in early 2000's**

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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  to des ... ck to
  neutra ...
  electron or photon interactions
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  to describe the excitation of atoms due to photon interaction

In ENDL format only

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**

First library managed by CSEWG (D. Brown) — IAEA (A. Trkov) collaboration

Usual ENDF Workflow

- **Version controlled with subversion** (ask me for access)
    - Full ENDF library
    - Use GForge
    - Have bug trackers, wiki etc
- **Phase 0 checking:** evaluator checks in, we check for legal ASCII, etc.
- **Phase 1 checking:** ADVANCE continuous integration system checks out data and does simple physics and format validation
- **Phase 2 checking:** Validation in user codes against macroscopic experiments
- **Release!**

U.S. DEPARTMENT OF ENERGY

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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

Formatting problems with EPICS

Content

Different content for different data formats

Not trivial to retrieve what contains what

EADL

Physics Data	EADL91 ENDL	EADL91 ENDF-6	EPICS2014 ENDL	EPICS2014 ENDF-6	EPICS2017 ENDL	EPICS2017 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

EPDL

Physics Data	EPDL97 ENDL	EPDL97 ENDF-6	EPICS2014 ENDL	EPICS2014 ENDF-6	EPICS2017 ENDL	EPICS2017 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

EEDL

Physics Data	EEDL91 ENDL	EEDL91 ENDF-6	EPICS2014 ENDL	EPICS2014 ENDF-6	EPICS2017 ENDL	EPICS2017 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

First validation test

Electron ionisation cross sections

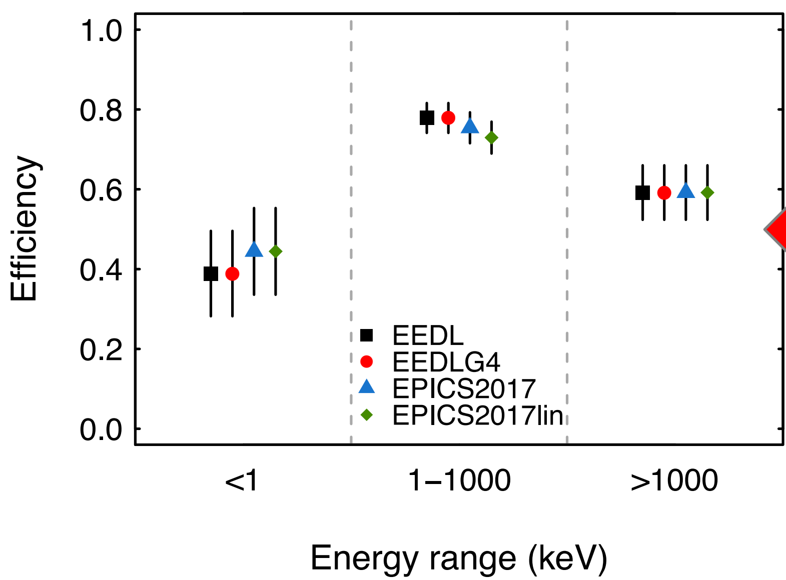
~ 2800 K shell cross section measurements

efficiency = fraction of test cases where H0 is not rejected

Goodness-of-fit tests

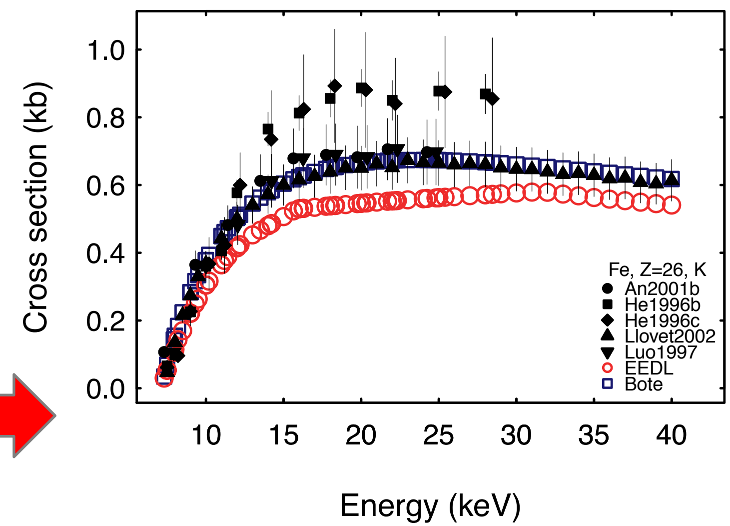
- χ^2
- Anderson-Darling
- Cramer-von Mises
- Kolmogorov-Smirnov

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!



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

We need better options for validating electro- or photo- atomic data

- Shielding benchmarks?
- **Lockwood energy deposition experiment**
- Hanson angular scattering
- Tabata charge deposition
- …

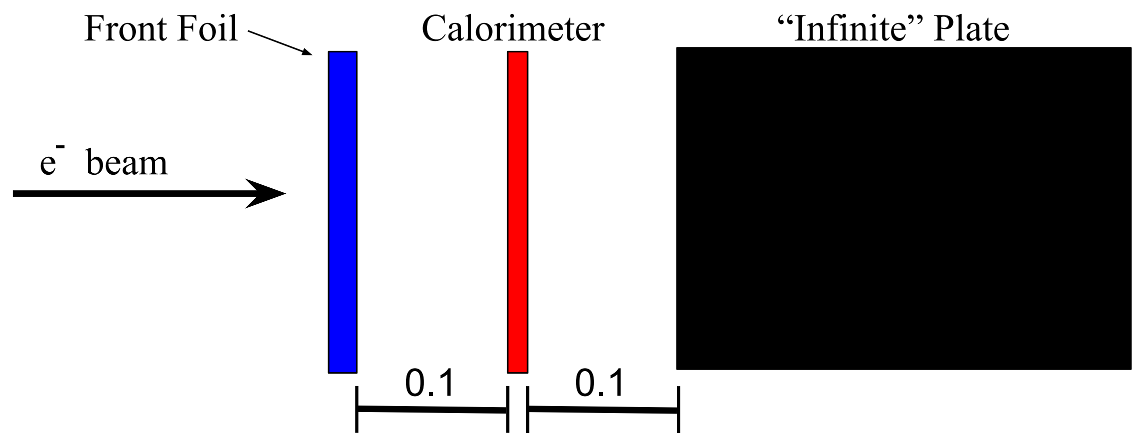


Fig. 2. The experimental setup of the Lockwood experiment consisting of a front foil, calorimeter foil, and "infinite" plate all of the same material and contained in vacuum.

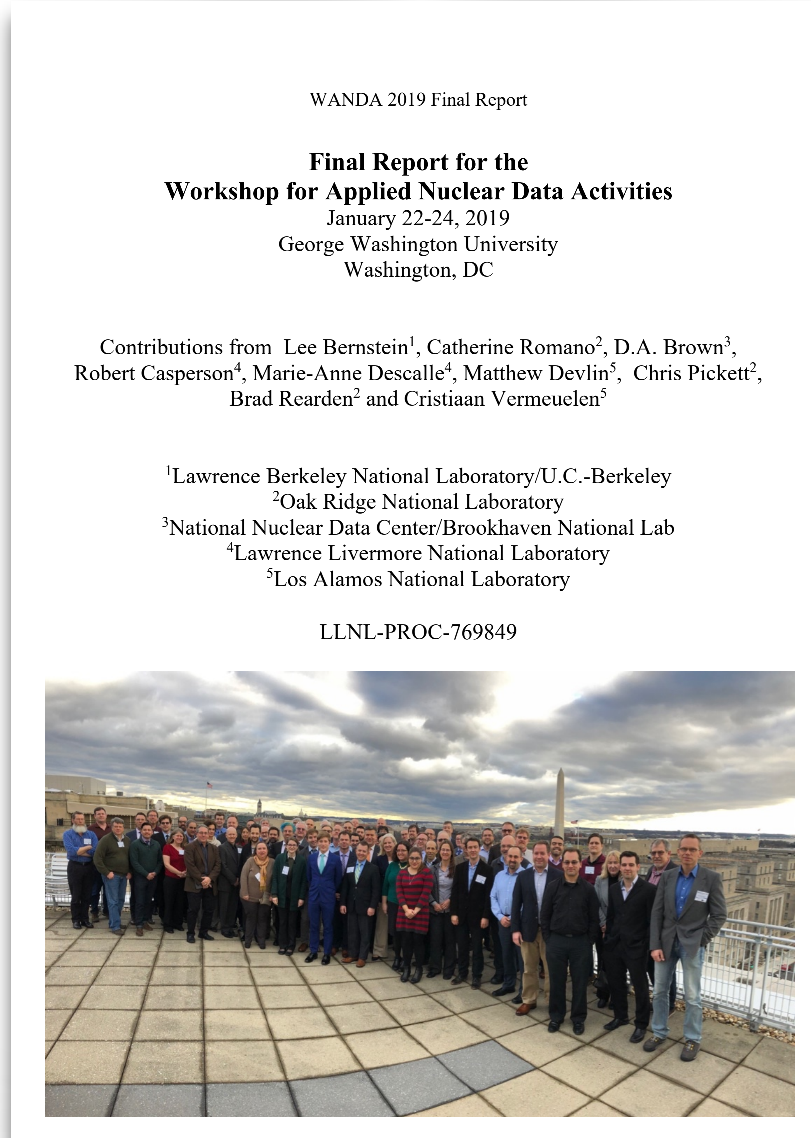
L. Kersting, D. Henderson, A. Robinson, E. Moll, ANS RPSD 2018–20th Topical Meeting of the Radiation Protection & Shielding Division of ANS, Santa Fe, NM, August 26–31, 2018, on CD-ROM, American Nuclear Society, LaGrange Park, IL (2018)

Status of CSEWG collaborations support of ENDF atomic data

- **CSEWG owns ENDF**
  - But 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

These gaps also identified in the WANDA2019 white paper

- We need people to maintain & improve the data
- We need people to test the data
- We need to identify ALL the users so we can get feedback


WANDA 2019 Final Report

Final Report for the
Workshop for Applied Nuclear Data Activities
January 22-24, 2019
George Washington University
Washington, DC

Contributions from Lee Bernstein[1], Catherine Romano[2], D.A. Brown[3], Robert Casperson[4], Marie-Anne Descalle[4], Matthew Devlin[5], Chris Pickett[2], Brad Rearden[2] and Cristiaan Vermeuelen[5]

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[3]National Nuclear Data Center/Brookhaven National Lab
[4]Lawrence Livermore National Laboratory
[5]Los Alamos National Laboratory

LLNL-PROC-769849

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Bright spots

- **Although processing with legacy codes is a forgotten art, we are developing new formats and processing codes**
    - New Generalized Nuclear Database Structure (GNDS) format:
        - Improved fidelity to physics
        - Addition of covariance data
        - Several open source Python & C++ API's available
    - Welcome input from users & experts
    - Developing under framework of NEA Working Party of Evaluation Cooperation groups
- **Hunting for users and potential developers to engage**
    - RPSD-2018
    - WANDA-2019 & planned in WANDA-2020
    - IEEE NSS-MIC 2019
    - Here!