Status of the Generalized Nuclear Database Structure (GNDS)

D. Brown, National Nuclear Data Center, BNL

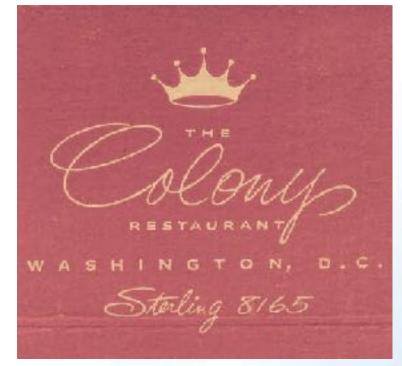


a passion for discovery



Before the ENDF format

- By 1960, there were many data efforts worldwide
 - different formats
 - often hard-coded libraries
 - proprietary data
 - Notable efforts: UKNDL (AWE, UK), NDA library (US), ENDL (LRL, US)
- ~1962 H. Honeck (BNL), A. Henry (Westinghouse), G. Joanou (GA) met at Colony Restaurant in DC decided on action
 - requested Reactor Mathematics and Computation Division of ANS sponsor 2 meetings to link databases



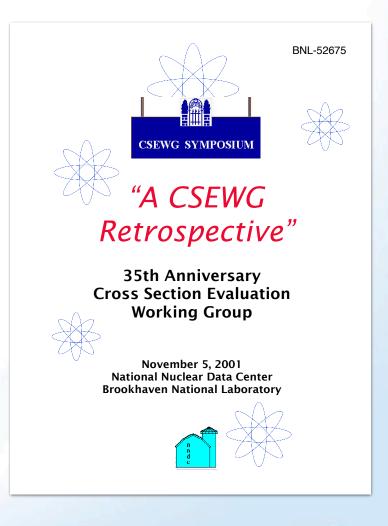
http://www.streetsofwashington.com/2013/10/fine-dining-inwashington-dc-in-1950s.html



2 NATIONAL LABORATORY

The first ENDF formats

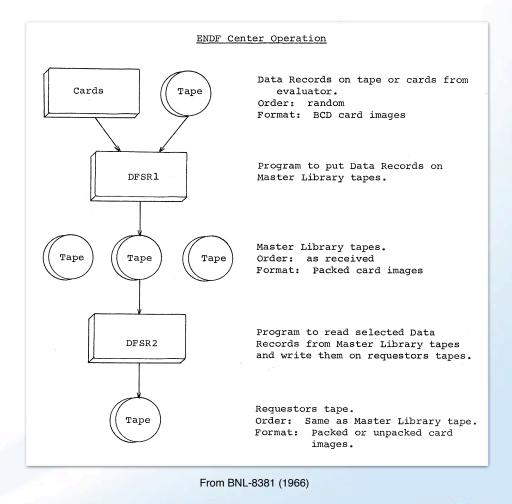
- ENDF/A documented in BNL-8381, released in 1965, based on UK's UKNDL with data from other libraries
- ENDF/B first documented in ENDF-102 (1966)
- ENDF/B-I library released in July 1968
 - Back then there was no "I", who would have predicted 50 years later we'd be releasing version "VIII.0"
- Original data project funded by Atomic Energy Commission in US





ENDF format was (and still is) tied to original infrastructure

- Original format designed to fit on IBM 80 column punchcards
 - Evaluations actually were occasionally submitted on punchcards
- Original data stored on magnetic tapes
- It was possible to request ENDF data on tapes and/or punchcards
 - Punchcard format was discouraged, BNL was trying to phase them out





This is an IBM 80 column punchcard

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https://en.wikipedia.org/wiki/Punched_card#/media/File:Blue-punch-card-front-horiz.png



This is a chunk of the n+59Co evaluation: it's punchcard-ready

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-5.000000+3	4.000000+0	1.898100+2	1.868200-1	0.00000+0	0.000000+02725	2151	7
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-2.258800+2	3.000000+0	9.164400+0	5.214100-2	0.000000+0	0.000000+02725	2151	9
1.320000+2	4.000000+0	5.270100+0	4.700000-1	0.000000+0	0.000000+02725	2151	10
4.323100+3	4.000000+0	1.041400+2	4.173700-1	0.00000+0	0.000000+02725	2151	11
5.016000+3	3.000000+0	6.789601+2	1.332200+0	0.000000+0	0.000000+02725	2151	12
6.389700+3	4.000000+0	1.681100+0	3.155600-1	0.000000+0	0.000000+02725	2151	13
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ENDF is resilient

- Death of Colony Restaurant in 1963
- AEC created CSEWG and ENDF; AEC ended in 1974, replaced with DOE in 1977
- ENDF/B-V made "classified", then unclassified
- Management of CSEWG by DOE "faded away" in the 1990's, but we kept going
- Internet revolution(s)
- 10 US Gov't administrations (including Trump)
- 50th (-ish) anniversary this year



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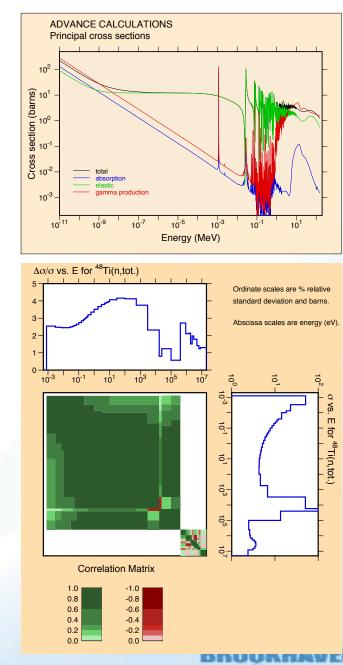
"It's a fantastic design, but I'm worried that after the games it'll just end up as a useless load of stone with no legacy potential."



The most important part of ENDF is the ecosystem built on the format

- PREPRO
- NJOY
- NNDC checking codes
- AMPX
- CALENDF

These are the tools that get the data into user's hands



FUDGE & GND history: an opportunity

- LLNL wanted to replace ENDL format (starting ~2005)
 - Decided against ENDF-6 and for a new structure: GND
 - ARRA funding made it possible
- Common re-design of format proposed to U.S. CSEWG (2011)
 - BNL/LANL/ORNL
- Common re-design of format proposed to NEA-WPEC — Led to SG38 (2012-2016)
 - Focus on redesigning structure and infrastructure
- Work will continue in SG-43 (2017-2020) and EG-GNDS (2017 onwards)



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Task of SG38: design and document a modern replacement for the ENDF-6 format

- Generalized Nuclear Database Structure (GNDS)
- Initial design is nearly complete, will be finished prior to ENDF-VIII release
 - Remaining changes are driven by new types of data accepted into ENDF-6 format
- After ENDF-VIII release, oversight of GNDS passes to a long-term WPEC subgroup that will review proposed format changes / additions



SG38 is finishing GNDS documentation

Documents, completed and still being finalized:

- Requirements for organizing data in the new structure
- Specifications for organizing data
- Requirements and specifications for general-purpose data containers
- Requirements and specifications for documentation sections
- Requirements and specifications for storing particle data
- All documents available from NEA website:
 - https://www.oecd-nea.org/science/wpec/sg38/



New subgroup (SG43) builds on SG38, designing tools to promote use of GNDS

- Tasks include defining a standard API for accessing data from GNDS files, and using the API to start implementing data quality checks
 - similar to FIZCON, PSYCHE, etc. for ENDF-6
- For more details see SG43 websites
 - <u>https://www.oecd-nea.org/science/wpec/sg43/</u> (official NEA website)
 - <u>https://github.com/GeneralizedNuclearData/SG43/wiki</u> (collaboration space)



GNDS files include particle data: mass, excited levels, halflives, decay information etc.

- Properties of Particles (PoPs) section was designed to handle the types of particle data in ENDF
 - Reaction sub-libraries include masses, spins, gamma-decay info
 - Decay sub-library includes general decay information such as discrete and continuum radiation
 - Fission yield sub-libraries
- Early goal of SG38 was to extend PoPs to also handle ENSDF-style evaluations. Not yet achieved, but may still be possible
 - Need more feedback and suggestions from ENSDF community to proceed



WPEC Subgroup 43

Mandate

Code infrastructure to support a general nuclear database structure to aide in international adoption.

Needs:

- An Application Programming Interface (API) for reading and writing data in GNDS
- Checking codes to help validate new evaluations

https://github.com/GeneralizedNuclearData/SG43

Physics Checking

- Develop list of physics rules to check
- Adopt severity levels and specify their meaning
- Develop standardized way of reporting errors

API Design

- API vs. implementation
- Begin initial API details
- Begin with low-level API to abstract away file details
- Establish naming conventions

- 1. Prioritize list of physics rules
- Write just enough API/implementation to be able check first
 2–3 rules
- 3. Write checking code that uses API/implementation to perform first 2–3 checks
- 4. Checking code success/failure will inform how well API/implementation is fulfilling needs.
- 5. Repeat ad nauseam

Where we are now

- "New management": SG-38, SG-43, EG-GNDS
- De-facto reference implementation:
 - FUDGE-4.2.2 Released June 2017
 - GND-1.8 Released June 2017
 - Plan at least one more release before B-VIII.0
 - Changes managed by EG-GNDS afterwords

Documentation:

- Requirements BNL report BNL-112394-2016-IR
- Complete format specifications due 2017
- ENDF/B-VIII, JEFF-4 to be released in both ENDF/B-6 and GND formats



GND Highlighted in LLNL's Sep. 2016 issue of Science & Technology Review

Most importantly: a new code ecosystem is developing thanks to the cooperation of the international data community