Perspectives and future of WPEC: SG38, SG43 and EG-GNDS

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a passion for discovery

U.S. DEPARTMENT OF ENERGY | Office of Science

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

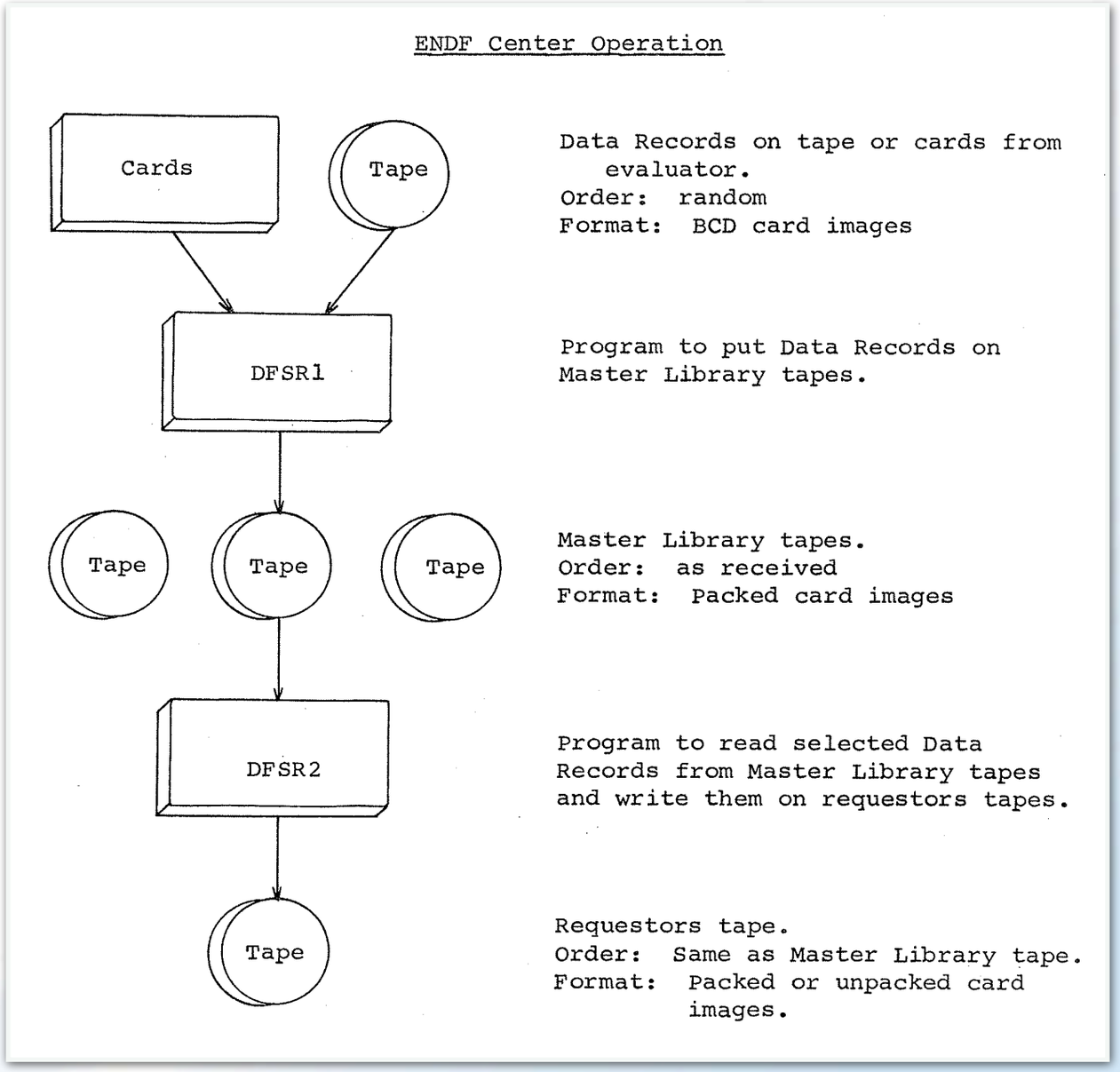
http://www.streetsofwashington.com/2013/10/fine-dining-in-washington-dc-in-1950s.html

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

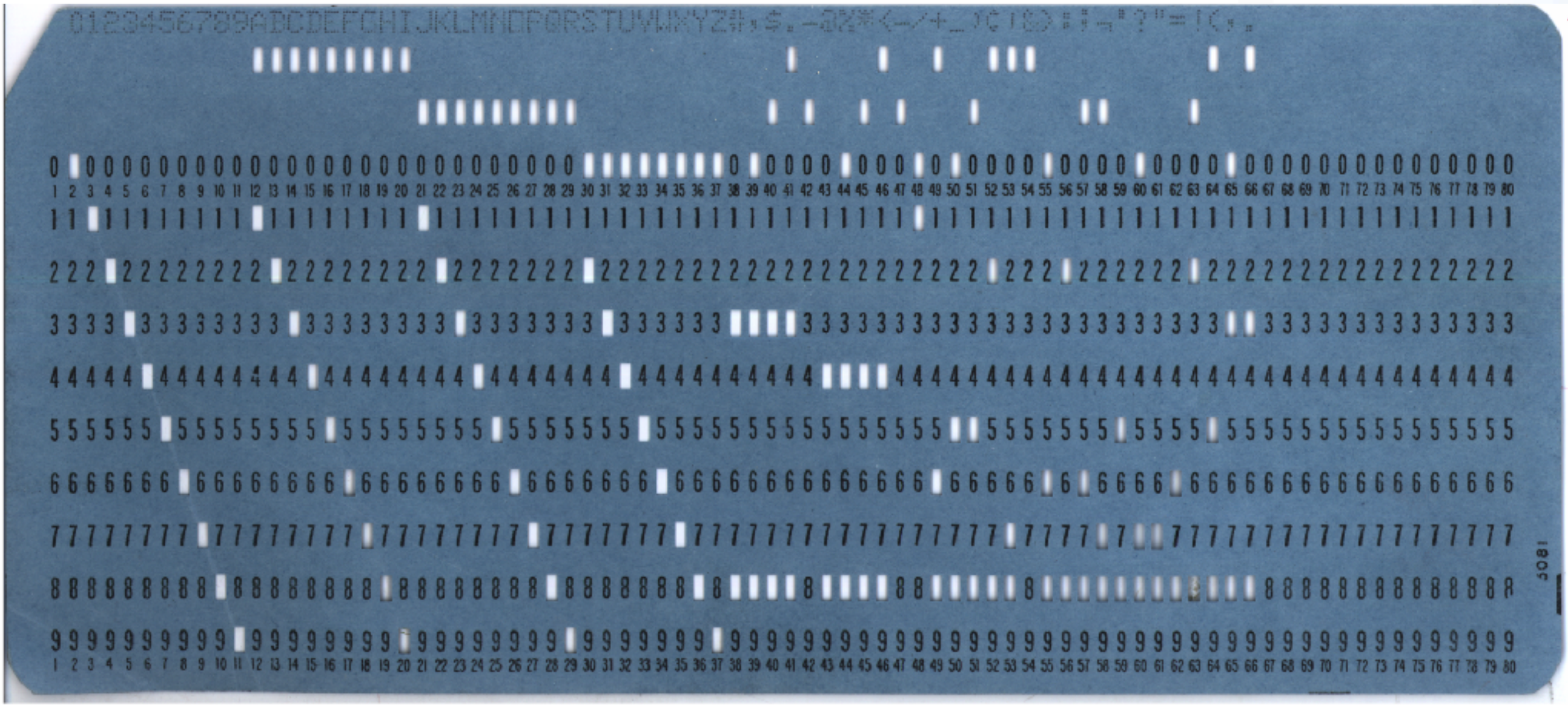
ENDF format was (and still is) tied to original infrastructure

- **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



From BNL-8381 (1966)

This is an IBM 80 column punchcard



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

```
                                 14          83           1          02725 1451   286
                                 14          84           1          02725 1451   287
                                 14          85           1          02725 1451   288
                                 14          86           1          02725 1451   289
                                 14          87           1          02725 1451   290
                                 14          88           1          02725 1451   291
                                                                      2725 1  099999
                                                                      2725 0  0     0
 2.705900+4 5.842690+1           0           0           1          02725 2151     1
 2.705900+4 1.000000+0           0           0           1          02725 2151     2
 1.000000-5 1.000000+5           1           3           0          12725 2151     3
 3.500000+0 6.672000-1           0           0           2          32725 2151     4
 5.842690+1 6.672000-1           0           0         600        1002725 2151     5
-5.000000+3 3.000000+0 5.576800+2 9.215100+0 0.000000+0 0.000000+02725 2151     6
-5.000000+3 4.000000+0 1.898100+2 1.868200-1 0.000000+0 0.000000+02725 2151     7
-4.767000+2 4.000000+0 1.949000-2 2.148900+0 0.000000+0 0.000000+02725 2151     8
-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 0.000000+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
```

ENDF is resilient

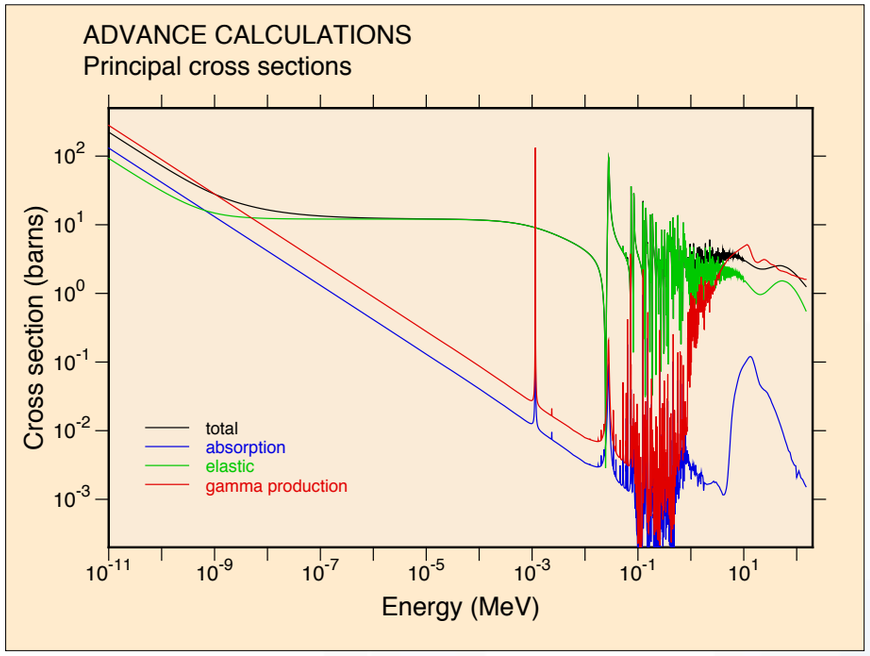
- Death of Colony Restaurant in 1963
- AEC created CSEWG and ENDF; AEC ended in 1974, replaced with DOE in 1977
- ENDF/B-V made “classified”, then unclassified
- Management of CSEWG by DOE “faded away” in the 1990’s, but we kept going
- Internet revolution(s)
- 10 US Gov’t administrations (including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

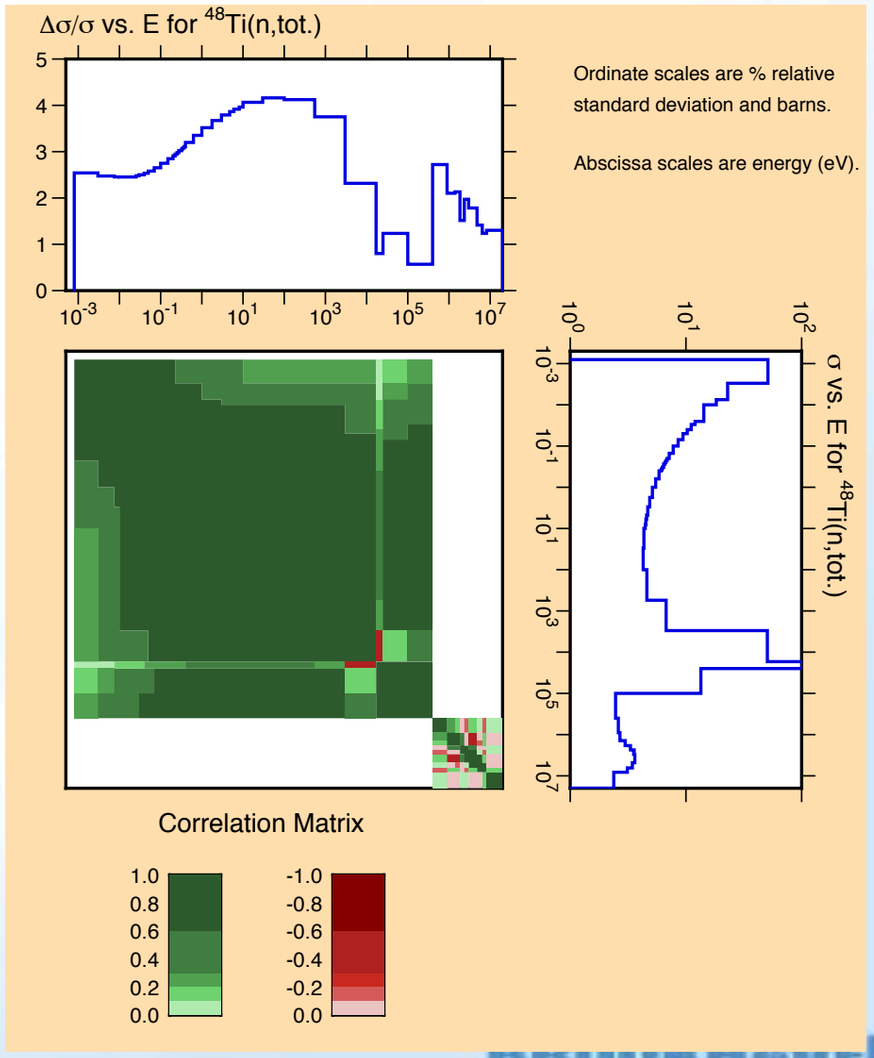
“It’s a fantastic design, but I’m worried that after the games it’ll just end up as a useless load of stone with no legacy potential.”

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

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

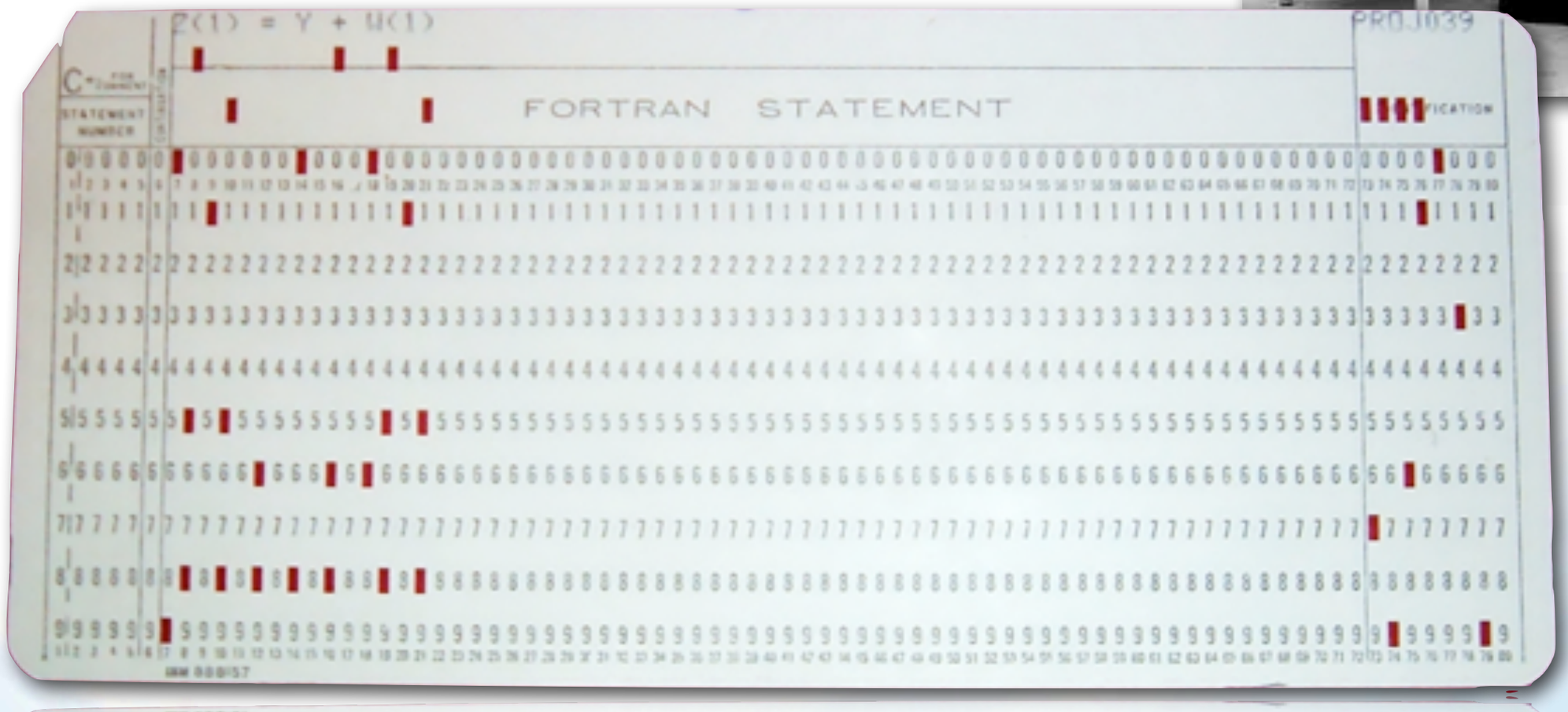
These are the tools that get the data into user's hands





Legacy formats

…but will we continue to be enslaved by this “modern technology”?



Slide based on slide from M. Herman

No, seriously

- A good format can determine the data structures used to interact with it
- These data structures are the components we use to create new things
- **We are trying to create a development environment (tools + components) that we enjoy working with**
- We will be working with these tools for a long time

Good tools == Happy developers

ENDF is resilient, but…

- **Obsolete (and therefore confusing) constructs**
  - FEND, MEND, SEND and TEND “cards”
  - line numbers (for the punchcards)
- **Limitations imposed by original physical format**
  - Fixed precision
  - Limited MT’s
  - Limited MAT’s
- **“Design by committee”**
  - MF6
  - Fission data in MT1 not MT18
  - Resonances
  - …
- **“Not fun to work with”, is often is barrier for newcomers**

The biggest danger are the legacy tools becoming “black boxes”

- **Original developers are deceased, retired or soon to retire**
  - NJOY (LANL)
    - McFarlane retired
    - Kahler retiring in June
  - PREPRO (IAEA)
    - Cullen retired
  - ndfgen/mcfgen (LLNL)
    - Perkins deceased
  - AMPX (ORNL)
    - Greene retired
  - CALENDF (CEA)
    - Ribon retired
  - NNDC codes (BNL)
    - Dunford deceased
- **“if it ain’t broke, don’t fix it”, but…**
- **We must understand how these codes work otherwise be become little more than a cargo cult**

A gritty reboot of the ENDF franchise

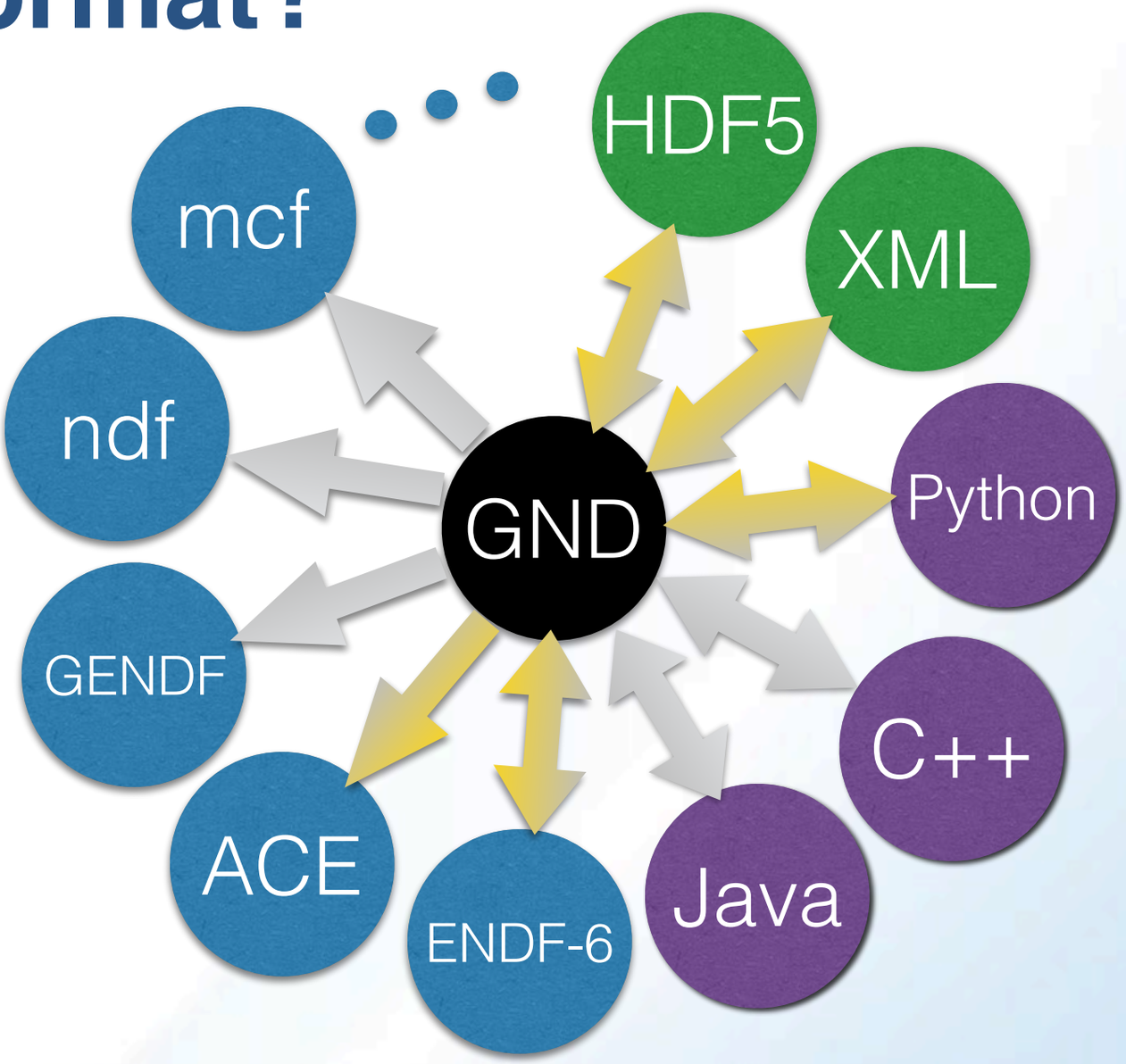
- **Want to preserve the evaluators' intent; but bad format meant evaluators put things in places they don't belong**
  - pseudo levels in 6,7Li (ab)used in MF4, before MF6 developed
  - fission in W
  - "battle over MT's" for high energy reactions
  - gammas in MT3 or 4 rather than with the reaction that produced them
  - …
- **Bad design leads to mistakes, want to engineer them away**
  - Backgrounds in resonance region
  - Multiple ways to store the same thing (gammas in MF12,13,14 vs. gammas in MF6), possible double counting
  - Synchronization issues (masses, levels, …)
  - …

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**
  - SG38 (2012-2016)
  - Focus on redesigning structure and infrastructure
- **Work will continue in SG-43 (2017-2020) and EG-GNDS**

What do (did?) we want to get out of the new format?

- **Both human and computer readable**
  - A textual representation → XML
  - A binary representation → HDF5
- **Extensible**
  - Adding a “new” section should not break any reading code
- **Handle legacy data**
  - Read & possibly correct data
  - Maintain high quality of libraries
- **Make provisions for both evaluated and processed data**
  - Support multiple representations simultaneously (and their dependence)
  - Ex. Resonance parameters and reconstructed pointwise cross sections (0K) and heated cross sections etc.



The work was divided into several sub-tasks

1. Top-level hierarchy for storing nuclear reaction data
2. Hierarchy for storing particle/nucleus data
3. Low-level data containers
4. API for reading and writing data in the new structure
5. Infrastructure for data handling, processing, plotting, etc.
6. Defining the tests that will be needed to assure quality of data
7. Governance

SG-38
Mostly done

SG-43
2017-2020

EG-GNDS

Slide based on slide from F. Malvagi

WPEC-SG38 (2012-2016)

- **Coordinator: D. McNabb (LLNL)**
- **2 Meetings/year (public)**
  - At the NEA (Paris), but also at JAEA, BNL, IAEA
  - 20/30 participants
- **From a wide range of Countries …**
  - AUT, CAN, CHN, DEU, FRA, GBR, JPN, KOR, RUS, SVN, USA,
- **... and Institutions ...**
  - International: NEA, IAEA
  - U.S.: LLNL, BNL, LANL, ORNL, NCSU, ...
  - Europe: CEA, IRSN, KIT, CCFE, KI, JSI, ...
  - Asia: JAEA, KAERI
- **... and Data Projects**
  - ENDF, JEFF, JENDL, ENSDF, EXFOR, RIPL

Slide based on slide from F. Malvagi

The follow-on groups

- **SG-43's mission is to develop an API for GNDS**
  - First meeting was yesterday
  - In 3 years, goal to have API specifications drafted
  - Stretch goal: actual implementation of API
- **Wait, did you say GNDS?**
  - Yeah, NEA management renamed the format, it is now the Generalized Nuclear Database Structure (GNDS)
- **EG-GNDS is the expert group to oversee GNDS**
  - Governance
  - Documentation
  - Training & outreach

So what does GNDS look like?

A real example: ENDF/B-VIII.0β4's n+3Li

- **What I did:**
  - Installed FUDGE from svn repo (sorry, to be released ~ 1 month)
  - Translated `n-003_Li_007.endf` using `endf2gnd.py` in FUDGE

```
dbrown$ ~/Desktop/fudge/site_packages/bin/endf2gnd.py n-003_Li_007.endf
dbrown$ ls n-003_Li_007*
n-003_Li_007.endf  n-003_Li_007.endf.gnd.xml  n-003_Li_007.endf.gndCov.xml
```

  - Edit `n-003_Li_007.endf.gnd.xml` in TextWrangler
    - many web browsers, IDE's and text editors can syntax highlight too

This is a zoom into the MT=4, a redundant cross section (but very illustrative)

```
<crossSectionSum label="(z,n)" ENDF_MT="4">
  <summands>
    <add xlink:href="/reactionSuite/reactions/reaction[@label='n + (Li7_e1 -> Li7 + photon)']/crossSection"/>
    <add xlink:href="/reactionSuite/reactions/reaction[@label='n + (Li7_e2 -> H3 + He4)']/crossSection"/>
      .
      .
      .
    <add xlink:href="/reactionSuite/reactions/reaction[@label='n + (Li7_e32 -> H3 + He4)']/crossSection"/></summands>
  <Q>
    <constant1d label="eval" constant="-477610" domainMin="546277" domainMax="2e7">
      <axes>
        <axis index="1" label="energy_in" unit="eV"/>
        <axis index="0" label="Q" unit="eV"/></axes></constant1d></Q>
<crossSection>
  <XYs1d label="eval">
    <axes>
      <axis index="1" label="energy_in" unit="eV"/>
      <axis index="0" label="crossSection" unit="b"/></axes>
    <values length="268">
      5.46277000e+05 0.000000e+00 5.50000000e+05 5.906900e-03 6.00000000e+05 2.517300e-02 6.50000000e+05 3.828500e-02 7.00
      4.30000000e+06 3.166236e-01 4.40000000e+06 3.113517e-01 4.50000000e+06 3.080398e-01 4.60000000e+06 3.078901e-01 4.70
      1.11520000e+07 4.333788e-01 1.15000000e+07 4.259431e-01 1.17240000e+07 4.211807e-01 1.20000000e+07 4.154468e-01 1.22
    <uncertainties>
      <uncertainty type="covariance">
        <link xlink:href="/covarianceSuite/section[@label='(z,n)']"/></uncertainty></uncertainties></XYs1d></crossSection>
```

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      .
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      1.11520000e+07 4.333788e-01 1.15000000e+07 4.259431e-01 1.17240000e+07 4.211807e-01 1.20000000e+07 4.154468e-01 1.22
    <uncertainties>
      <uncertainty type="covariance">
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```

MF=4 obeys a sum rule in ENDF, I never remember what it is

```
<crossSectionSum label="(z,n)" ENDF_MT="4">
  <summands>
    <add xlink:href="/reactionSuite/reactions/reaction[@label='n
    <add xlink:href="/reactionSuite/reactions/reaction[@label='n
      .
      .
      .
    <add xlink:href="/reactionSuite/reactions/reaction[@label='n
```

- Says it is a sum
- Label has rational, human readable name
- Gives ENDF equivalent
- Lists explicitly reactions summed
- Provide URL of each summand

This is a zoom into the MT=4, a redundant cross section (but very illustrative)

```
<crossSectionSum label="(z,n)" ENDF_MT="4">
  <summands>
    <add xlink:href="/reactionSuite/reactions/reaction[@label='n + (Li7_e1 -> Li7 + photon)']/crossSection"/>
    <add xlink:href="/reactionSuite/reactions/reaction[@label='n + (Li7_e2 -> H3 + He4)']/crossSection"/>
      .
      .
      .
    <add xlink:href="/reactionSuite/reactions/reaction[@label='n + (Li7_e32 -> H3 + He4)']/crossSection"/></summands>
  <Q>
    <constant1d label="eval" constant="-477610" domainMin="546277" domainMax="2e7">
      <axes>
        <axis index="1" label="energy_in" unit="eV"/>
        <axis index="0" label="Q" unit="eV"/></axes></constant1d></Q>
<crossSection>
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    <uncertainties>
      <uncertainty type="covariance">
        <link xlink:href="/covarianceSuite/section[@label='(z,n)']"/></uncertainty></uncertainties></XYs1d></crossSection>
```

The cross section

```
<crossSection>
  <XYs1d label="eval">
    <axes>
      <axis index="1" label="energy_in" unit="eV"/>
      <axis index="0" label="crossSection" unit="b"/></axes>
    <values length="268">
      5.46277000e+05 0.000000e+00 5.50000000e+05 5.906900e-03 6.00000000e
      4.30000000e+06 3.166236e-01 4.40000000e+06 3.113517e-01 4.50000000e
      1.11520000e+07 4.333788e-01 1.15000000e+07 4.259431e-01 1.17240000e
    <uncertainties>
      <uncertainty type="covariance">
        <link xlink:href="/covarianceSuite/section[@label='(z,n)']"/></un
```

- <crossSection> is high level, <XYs1d> is low level (~TAB1)
- Units & label given in <axes>, guide for plotting
- <values> hold X-Y pairs, any precision, read left to right. Line feeds don't matter
- <uncertainty> too big, so give a URL pointing to the covariance file

This is a zoom into the MT=4, a redundant cross section (but very illustrative)

```
<crossSectionSum label="(z,n)" ENDF_MT="4">
  <summands>
    <add xlink:href="/reactionSuite/reactions/reaction[@label='n + (Li7_e1 -> Li7 + photon)']/crossSection"/>
    <add xlink:href="/reactionSuite/reactions/reaction[@label='n + (Li7_e2 -> H3 + He4)']/crossSection"/>
      .
      .
      .
    <add xlink:href="/reactionSuite/reactions/reaction[@label='n + (Li7_e32 -> H3 + He4)']/crossSection"/></summands>
  <Q>
    <constant1d label="eval" constant="-477610" domainMin="546277" domainMax="2e7">
      <axes>
        <axis index="1" label="energy_in" unit="eV"/>
        <axis index="0" label="Q" unit="eV"/></axes></constant1d></Q>
  <crossSection>
    <XYs1d label="eval">
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        <axis index="0" label="crossSection" unit="b"/></axes>
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        5.46277000e+05 0.000000e+00 5.50000000e+05 5.906900e-03 6.00000000e+05 2.517300e-02 6.50000000e+05 3.828500e-02 7.00(
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        1.11520000e+07 4.333788e-01 1.15000000e+07 4.259431e-01 1.17240000e+07 4.211807e-01 1.20000000e+07 4.154468e-01 1.22(
      <uncertainties>
        <uncertainty type="covariance">
          <link xlink:href="/covarianceSuite/section[@label='(z,n)']"/></uncertainty></uncertainties></XYs1d></crossSection>
```

Here Q is a constant, but it doesn't have to be (think fission)

```
<Q>
  <constant1d label="eval" constant="-477610" domainMin="546277" domainMax="2e7">
    <axes>
      <axis index="1" label="energy_in" unit="eV"/>
      <axis index="0" label="Q" unit="eV"/></axes></constant1d></Q>
```

- <Q> is a high level element
- <constant1d/> is a low level data container
- Gives value (-477610) units (eV) and labels
- Gives energy range over which this container valid (546277-2e7 eV)
- Yes, markup is overkill for a constant, but uniform arrangement means coding to read easier

GNDS's hierarchy is rational & easy to follow

```
<reactionSuite projectile="n" target="Li7" evaluation="ENDF/B-8.0" version="GND 1.7
  <styles> ••• </styles>
  <documentations> ••• </documentations>
  <PoPs name="protare_internal" version="1.0" format="PoPs 0.1"> ••• </PoPs>
  <resonances> ••• </resonances>
  <reactions>
    <reaction label="n + Li7" ENDF_MT="2">
      <crossSection> ••• </crossSection>
      <outputChannel genre="twoBody">
        <Q> ••• </Q>
        <products>
          <product name="n" label="n">
            <multiplicity> ••• </multiplicity>
            <distribution>
              <angularTwoBody label="eval" productFrame="centerOfMass"> ••• </angular
          <product name="Li7" label="Li7" ENDFconversionFlag="implicitProduct"> •••
```

Other handy features

- **File size typically smaller**
  - added size because of XML tags doesn't nearly match the bloat needed to support punchcards (line nums, MAT, MT, MF at ends of lines)
- **Processed data and evaluated data can live together in harmony, in the same file**
- **Files more readable**
  - Evaluators find it useful to edit ENDF files by translating to GND, hand editing, then translating back to ENDF (G. Nobre (BNL), I. Thompson (LLNL))
  - Syntax highlighting through most text editors, IDE's and web browsers
- **Open source format and tools**
  - Processing codes (FUDGE, NJOY2016, GRUCON) now useable by ALL, without $$$
  - Users find bugs and can send patches (common occurrence with FUDGE, NJOY now experiencing this benefit!)

FUDGE and GND(S) information are available in several places

- **https://www.oecd-nea.org/science/wpec/sg38/**
  - "Detailed requirements for a next generation nuclear data structure";
  - "Specifications for the next generation nuclear data hierarchy"
  - "Requirements and specifications for a particle database"
  - "General purpose data containers"
- **https://ndclx4.bnl.gov/gf/project/gnd/**
  - Fudge 4.2.1
    - Allows to translate ENDF-6 ↔ GND (V1.7)
- **http://www.nndc.bnl.gov/endf/b7.1/**
  - **ENDF/B-VII.1 translated into GND**
- **http://www.nndc.bnl.gov/endf & IAEA NDS**
  - **Built into ENDF retrievals**

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  - Fudge 4.2.1
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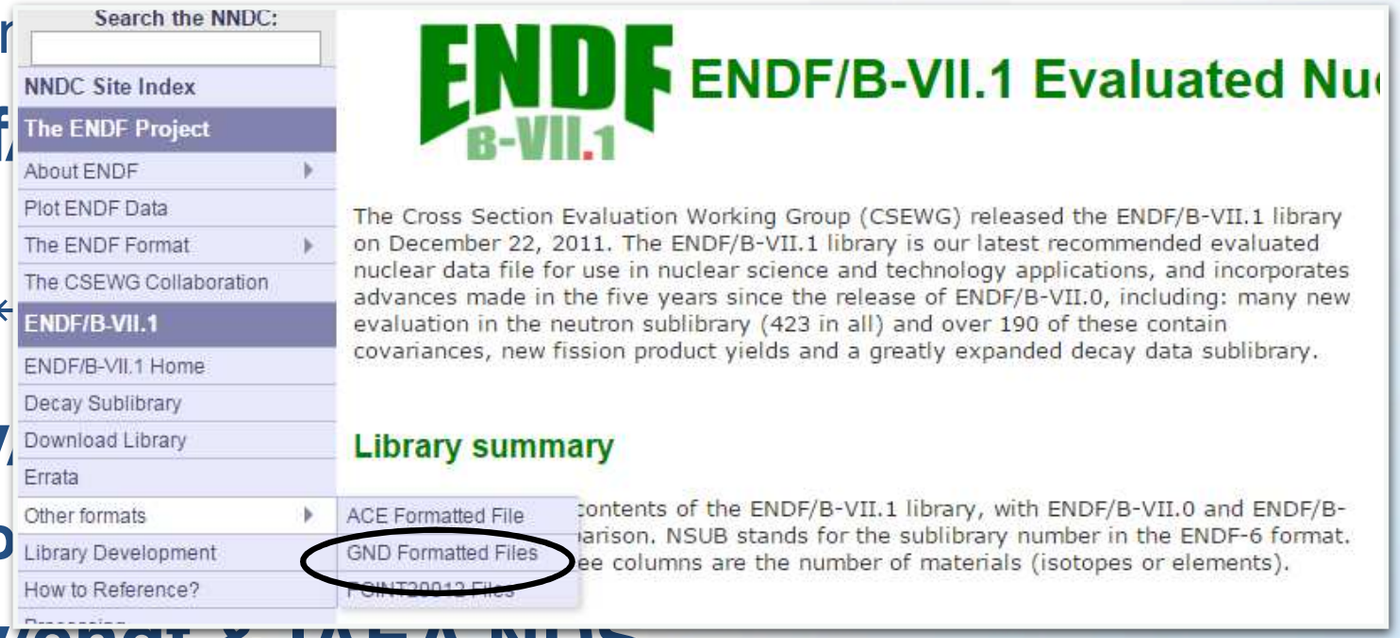
- **http://www.nndc.bnl.gov/**
  - **ENDF/B-VII.1 translated into**
- **http://www.nndc.bnl.gov/endf & IAEA NDS**
  - **Built into ENDF retrievals**



GND is under active development, stable version due with END/B-VIII.0 release

- **Standard transportable particles:**
  - alphas/
  - deuterons/
  - gammas/
  - helium3s/
  - neutrons/
  - protons/
  - standards/
  - thermal_scatt/
  - tritons/
- **Particle properties:**
  - atomic_relax/
  - decay/
- **Atomic physics:**
  - electrons/
  - photoat/
- **Fission product yields**
  - nfy/
  - sfy/

GND is under active development, stable version due with END/B-VIII.0 release

- ☑ **Standard trans… partic…**
  - ☑ alphas/
  - ☑ deuter…
  - ☑ gamma…
  - ☑ helium…
  - ☑ neutro…
  - ☑ protons/
  - ☑ standards/
  - ☑ thermal_scatt/
  - ☑ tritons/
- ☐ **Particle properties:**
- **…ics:**
- **…uct yields**
  - ☐ nfy/
  - ☐ sfy/

In addition to lots of tweaks…

We are also missing

URR probability tables

LB8 covariance

LRF=7 covariance

After ENDF/B-VIII.0, we will focus on new features

- **Improved documentation markup**
  - Unicode vs. Latex, Markdown
- **High energy data not limited by MT availability**
- **Syncing structure and reaction and decay data**
  - Simplifying cross-library data QA
  - Correlations (g-g are easiest to exploit)
- **New FPY format**
  - Q matrix, sync with decay data
  - Covariance
  - Common format (no special coding needed will be ready for ENDF/B-VIII.0)
- **New covariance formats**
  - Log-normal PDF
  - Various ways of decomposing a covariance matrix
- **New TSL format**
  - Relax several approximations

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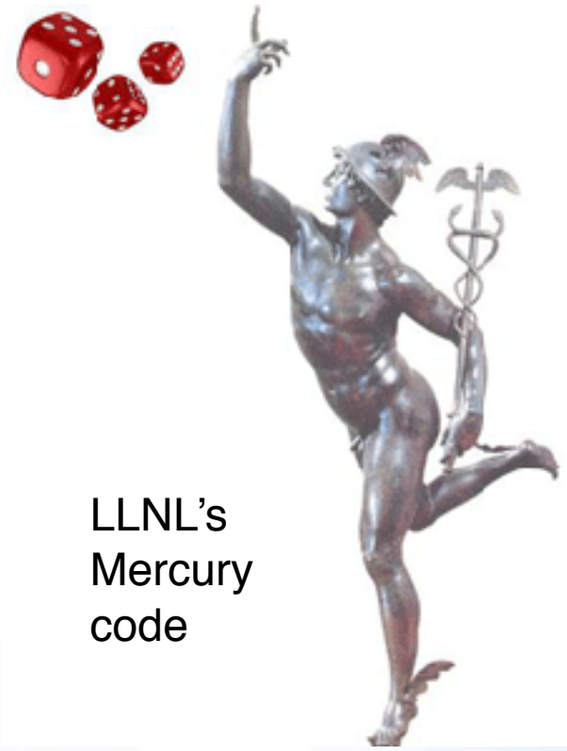
Some features already implemented

GND is *in production now*

- **GIDI: General Interaction Data Interface**
  - read and perform Monte Carlo sampling from GND-formatted data
  - implemented for LLNL Monte Carlo code MERCURY and GEANT4
  - Open Source
- **GEANT4: CERN high energy physics transport**
  - G4LND (old nuclear collision kernel)
  - G4LND/GIDI (GND format)



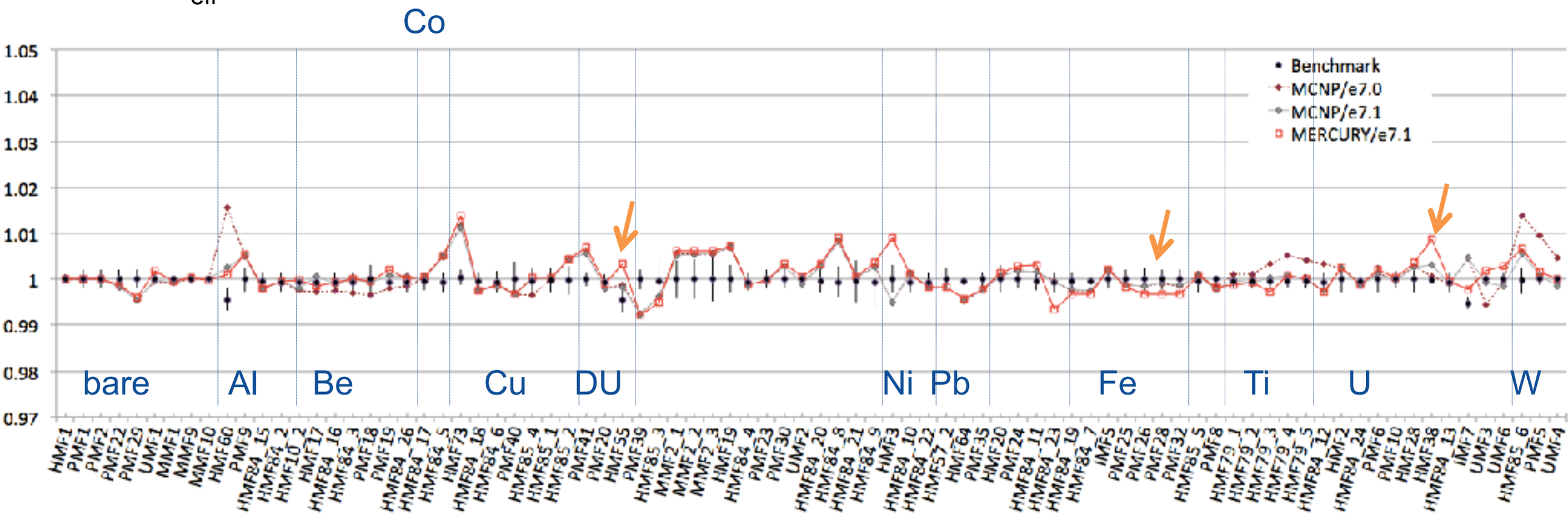
LLNL's Mercury code

- **MERCURY: LLNL all particle-transport Monte Carlo code**
  - MCAPM (old LLNL mcf format)
  - GIDI (GND format)
- **Data QA in ADVANCE**
  - plotting
  - inter
  - rigorous (and orthogonal) tests
  - since ENDF/B-VII.1 release (2011)
- **Ardra: LLNL deterministic transport**
- **Data visualization on NNDC & IAEA website**

ENDF/bVII.1 (GND)

M.-A. Descalle, ND2016

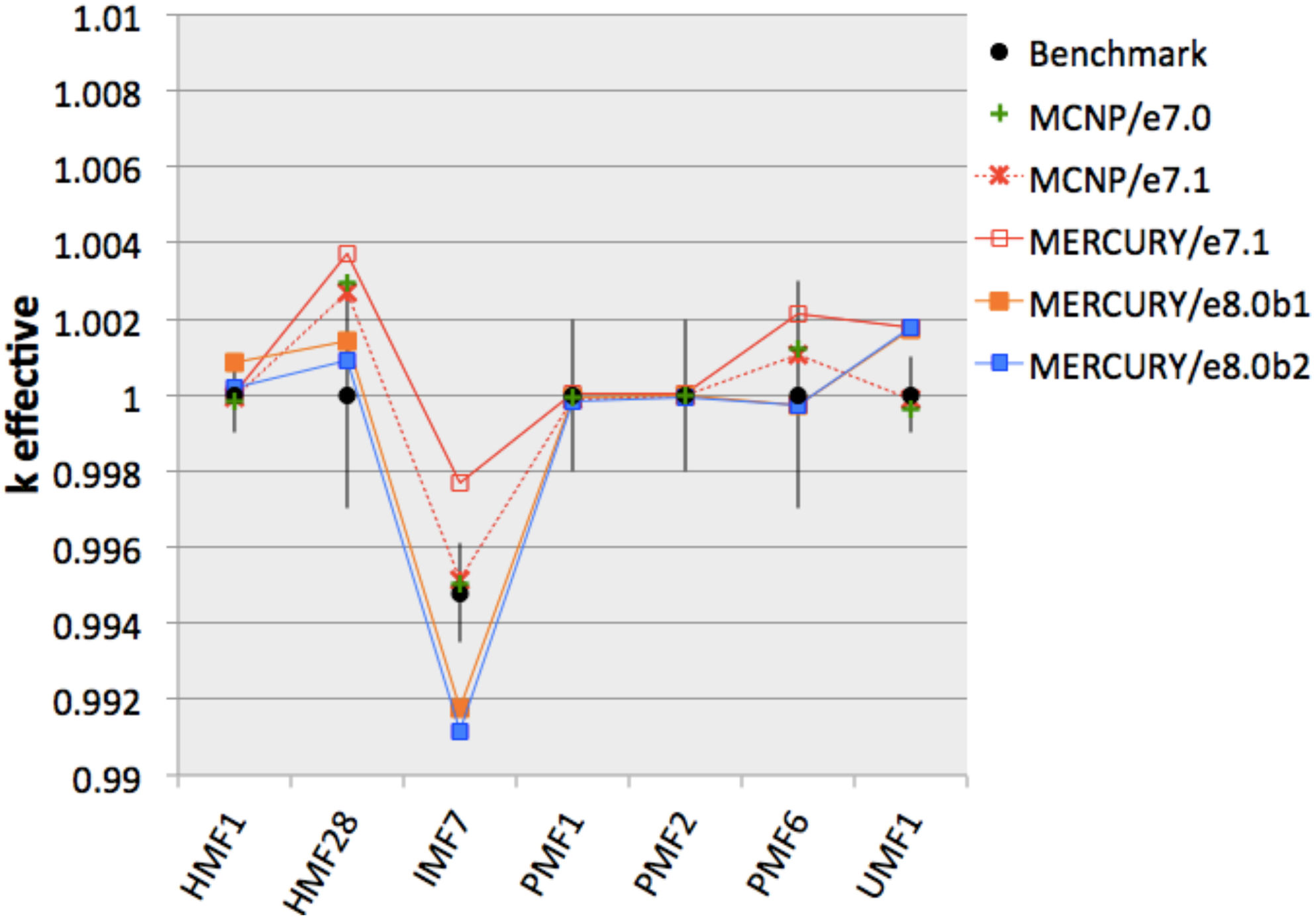
Ordinate: k_{eff}



ENDF/B-VII.1: MERCURY/GIDI results are in good agreement with MCNP results except for a few cases with U, Fe reflectors

Godiva, Jezebel, Jezebel240, Flattop25 & Pu, Big10

M.-A. Descalle, ND2016



Ongoing & Future Work

- GIDI is being implemented for LLNL Sn code Ardra, and V&V testing will start next month
- Angular biasing will be implemented in GIDI
  - TOF LLNL Pulsed Spheres
- FUDGE will translate data from GND to ACE format for comparison to MCNP results
- We will start testing reconstructed angular distributions within the next two months
- Following implementation, we plan to use criticality benchmark simulations to test:
  - Probability tables
  - Thermal scattering

Developers of processing codes actively working to implement GND

- **FUDGE (LLNL)**
  - First code to use GND
  - Open source, under BSD license
  - See https://ndclx4.bnl.gov/gf/project/gnd/
- **NJOY-21 (LANL)**
  - Long term, open source, replacement for NJOY2012
  - In active development, adding GND functionality
  - See https://njoy.github.io/
- **AMPX (ORNL)**
  - Being modernized as part of overall SCALE modernization effort
  - In active development, adding GND functionality
- **FRENDY (JAEA)**
  - GND support planned
- **GALILÉE (CEA)**
  - GND support planned
- **GAIA (IRSN)**
  - GND support planned
- **GRUCON (Kuchatov Inst.)**
  - GND support planned

SG-43 provides Open Source framework

Where we are now

- **"New management": SG-38, SG-43, EG-GNDS**
- **De-facto reference implementation:**
  - FUDGE-4.2.1 Released Mar. 2016
  - GND-1.7 Released Mar. 2016
  - 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