Database management for preparing for ENDF/B-VIII

D.A. Brown, NNDC

BROOKHAVEN NATIONAL LABORATORY

a passion for discovery

U.S. DEPARTMENT OF ENERGY | Office of Science

Outline

- ENDF/B-VII.2
- ENDF/B-VIII
- DOI issues
- ENDF website(s)

Outline

- **ENDF/B-VII.2**
- **ENDF/B-VIII**
- **DOI issues**
- **ENDF website(s)**

Details of an ENDF/B-VII.2 release
(as I see it)

- **Bug fixes**
  - Automated
  - Manual
- **An incomplete list of new/updated evaluations**
  - SiO_2, two phases MAT=47,49 (NCSU)
  - $^{63,65}Cu$ (ORNL)
  - $^{90\text{-}96}Zr$, Decay data fixes (BNL)
- **PR push/advertising**
  - Do we need a “Big Paper”?
  - Need to test that bug fixes didn’t cause trouble
  - Talks/meetings for announcing it
- **ENDF format for production; GND for testing**

Deficiencies noted by ADVANCE

http://www.nndc.bnl.gov/endf/b7.dev/qa/neutrons/reports/neutrons.html

Neutrons Sublibrary

ENDF/B Development Library

- General Information:
  - ENDF sublib designator: 10
- Revision Number: 611M
- Last Modified Revision: 532:611M
- Build Status:
  - Build status: ERROR
  - Build time: 2013-04-30 16:52:01.394282
  - Listfile: neutrons.list
  - Release Notes: neutrons-releaseNotes.pdf
- GForge Links:
  - Browse SVN
  - Browse sublibrary tracker

Latest Updates

sublib_release_notes: neutrons
Report sublib_release_notes on neutrons generated. The result was a SUCCESS
2013-04-30 16:57:39.661872

evaluation_summary: n-098_Cf_251.endf
Code evaluation_summary completed run on n-098_Cf_251.endf. The result was a SUCCESS
2013-04-30 16:52:41.503573

sublib_html: neutrons
Report sublib_html on neutrons generated. The result was a SUCCESS
2013-04-30 16:52:01.501892

Summary of all bugs

Periodic Table | Material List

Deficiencies noted by ADVANCE
(these are candidates for automatic fixing)

- **checkr** There is an error in an interpolation table for this data set: 2x
- **fizcon** All probability distributions should be normalized to 1, this one isn't.: 2x
- **fizcon** Data for a reaction started at a minimum Ein that is incorrect, based upon reaction's Q value.: 1x
- **fizcon** Outgoing energy E' not energetically allow: E' <= E-Q.: 7x
- **fizcon** The cross section and an outgoing distribution don't span the same energy region.:7x
- **fudge-4.0** Calculated and tabulated Q values disagree.: all of them
- **fudge-4.0** Calculated and tabulated thresholds don't agree: 28x
- **fudge-4.0** Energy doesn't balance: all of them
- **fudge-4.0** Energy range of data set does not match cross section range: 124x
- **fudge-4.0** Found a negative probability: 61x
- **fudge-4.0** Unnormalized outgoing probability distribution: most of them
- **njoy2012** An angular distribution is negative: 61x
- **njoy2012** Outgoing energy E' not energetically allow: E' <= E-Q.: 42x

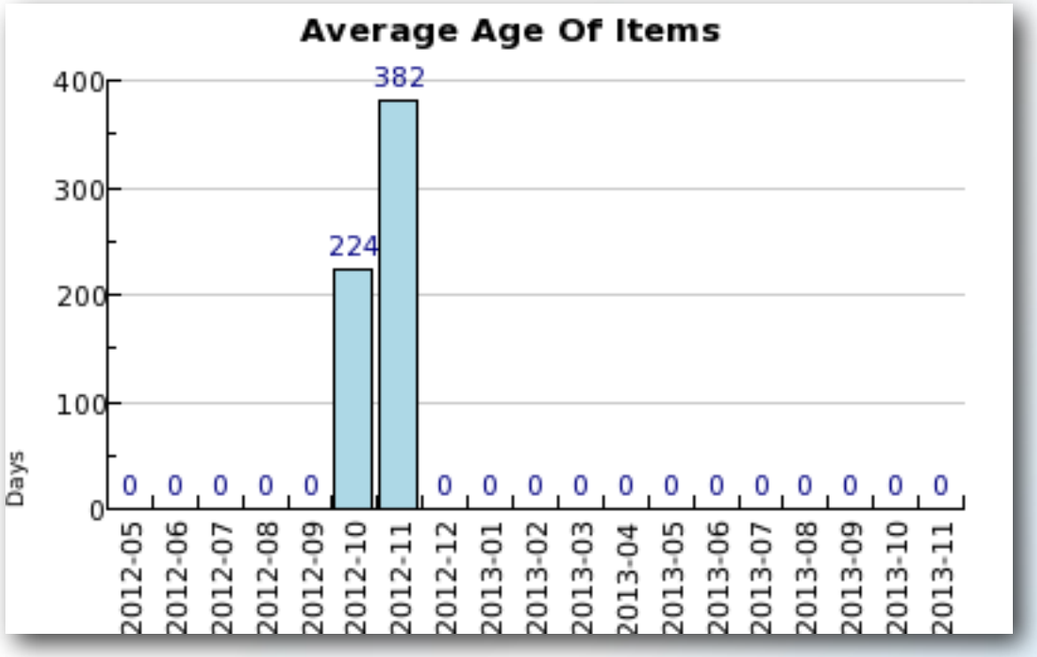
Possible automated fixes

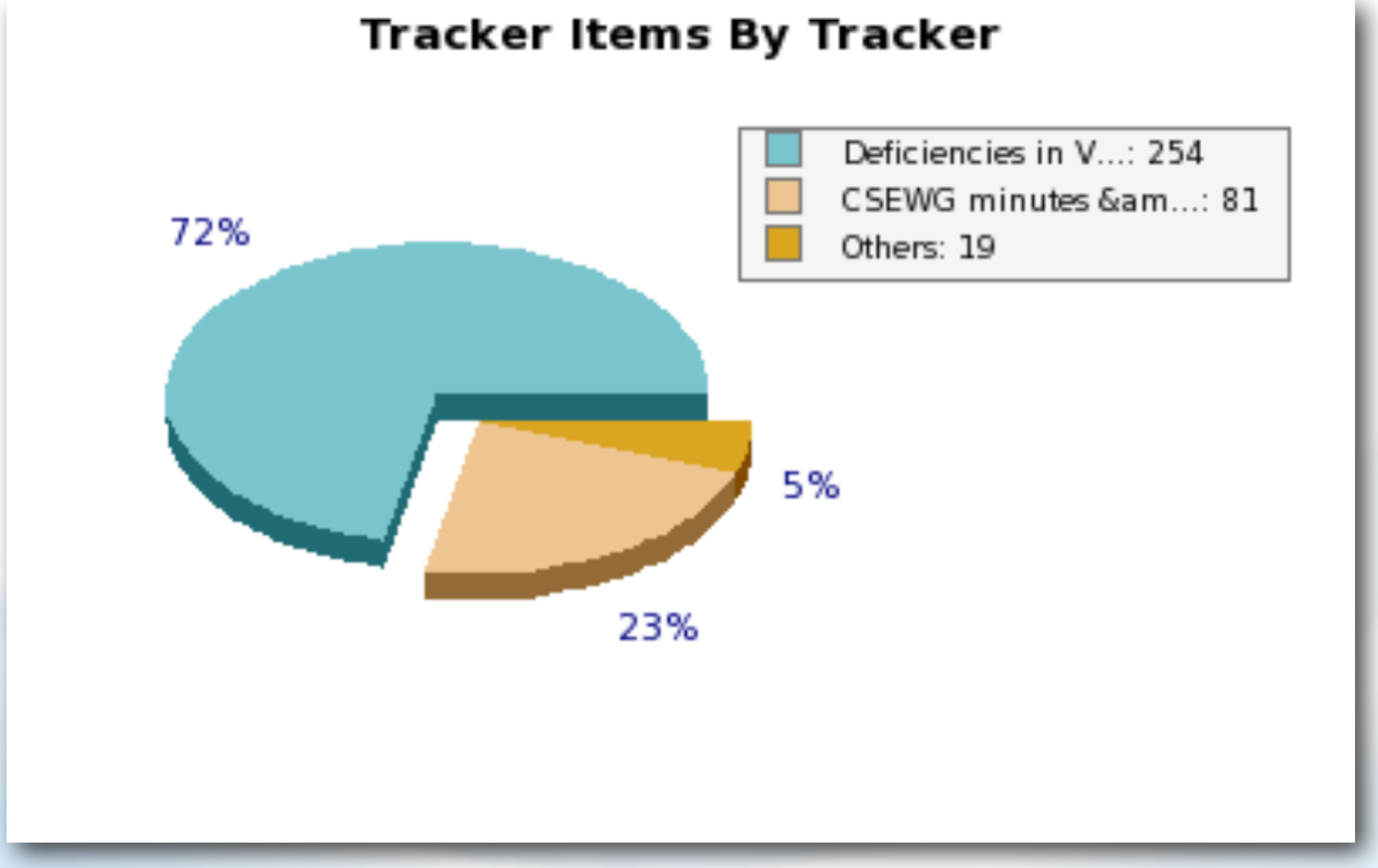
- **Mass related fixes:**
  - Sync masses,
  - Q values,
  - thresholds and
  - end-points of E’ spectra
- **Probability fixes:**
  - Normalizations of all probabilities
  - Put floor of zero on all probability distributions
- **Synchronize energy ranges between cross sections, distributions**
- **Line number removal**

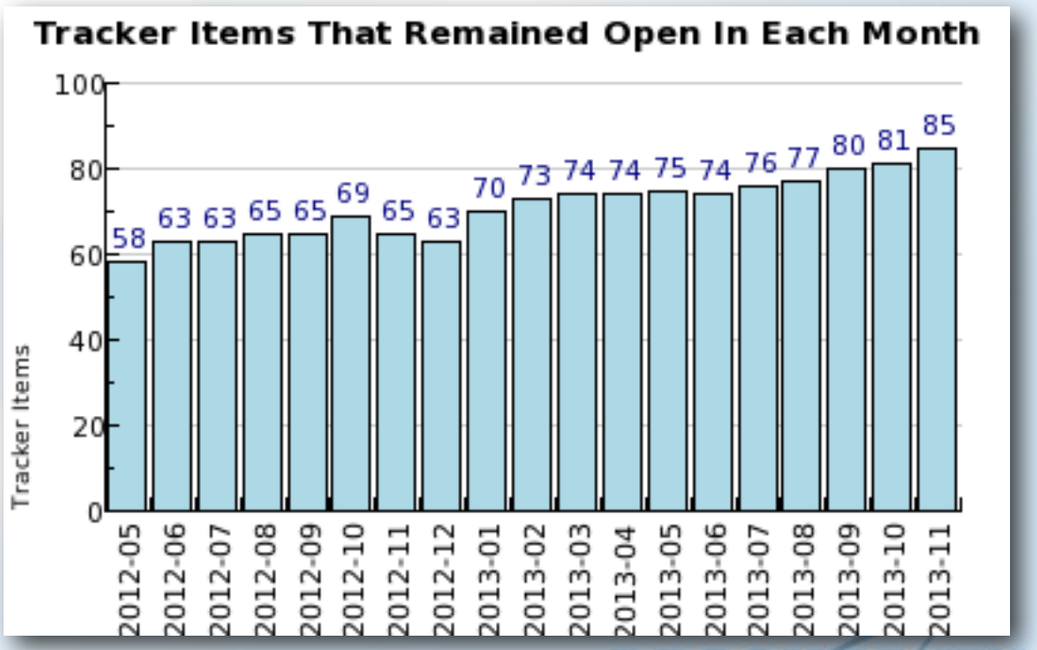
2-3 weeks effort to implement

Summary of current deficiencies in GForge

- A lot of activity for ENDF/B-VII.1
- Steady growth of number of bugs since







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Deficiencies in VII deuteron

• H-2: Energy range too short in the (d,n) reaction	2009-12-22 13:50:15

Deficiencies in VII decay

• Unspecified: Inconsistencies in half-lives	2009-12-22 13:53:21
• Unspecified: Fission beta-spectra 40% lower than in VI.8	2009-12-22 13:51:55
• Unspecified: Masses (AWR) inconsistent	2009-12-22 13:54:34
• Sb-129: Inconsistency in beta decay	2009-12-22 13:55:32
• Rh-102, Rh-102m: Warning statement in MT451	2009-12-22 13:56:46
• a problem with the Half-life of Rf-261 or Rf 261m in ENDF VII 1	2013-10-10 05:32:34
• Kr-90	2013-11-15 07:24:18

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• Ca-40, Cu-63: Inconsistent energy ranges in MF3 and MF6	2009-12-22 13:48:37
• Pb207 outgoing energies out of order	2012-03-09 17:44:26

Deficiencies in VII thermal scattering

• O in BeO, U in UO2: MAT numbers for thermal scat.	2009-12-22 13:45:02
• H in H2O: Wrong ZA value	2009-12-22 13:46:04
• U(UO2) and O(UO2) reversed	2012-07-10 13:36:07

Deficiencies in VII fission product yields (FPY)

• 241Pu in the rare earth region	2012-09-13 11:40:52
• As-84m doesn't exist, but we have a fission yield for it	2012-09-13 11:43:54
• FPY has non-existent metastable states	2013-09-21 05:43:57

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- Be7: Incomplete evaluation
- U-235,238,Pu-239: Too coarse fission spectra
- Eu-153: Negative distributions
- Mg-26, S-34, K-39: Problems with energy balance
- Mo-100: Unphysical peak in MF5 MT91
- Np-237: Thermal value to be updated
- Sn-122, Sn-120: Neutron widths of resonances
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- 229Pa level scheme incorrect
- remove redundant MF3 in RRR
- modify parameters for 1st resonance in U-236
- 50V, 49Ti, 65,67,68,70Zn and 93Nb have probability tables with incorrect normalization
- 240Pu(n,el) thermal cross section is very low
- Neutron outgoing energy too high for MF=5 files in 40Ar
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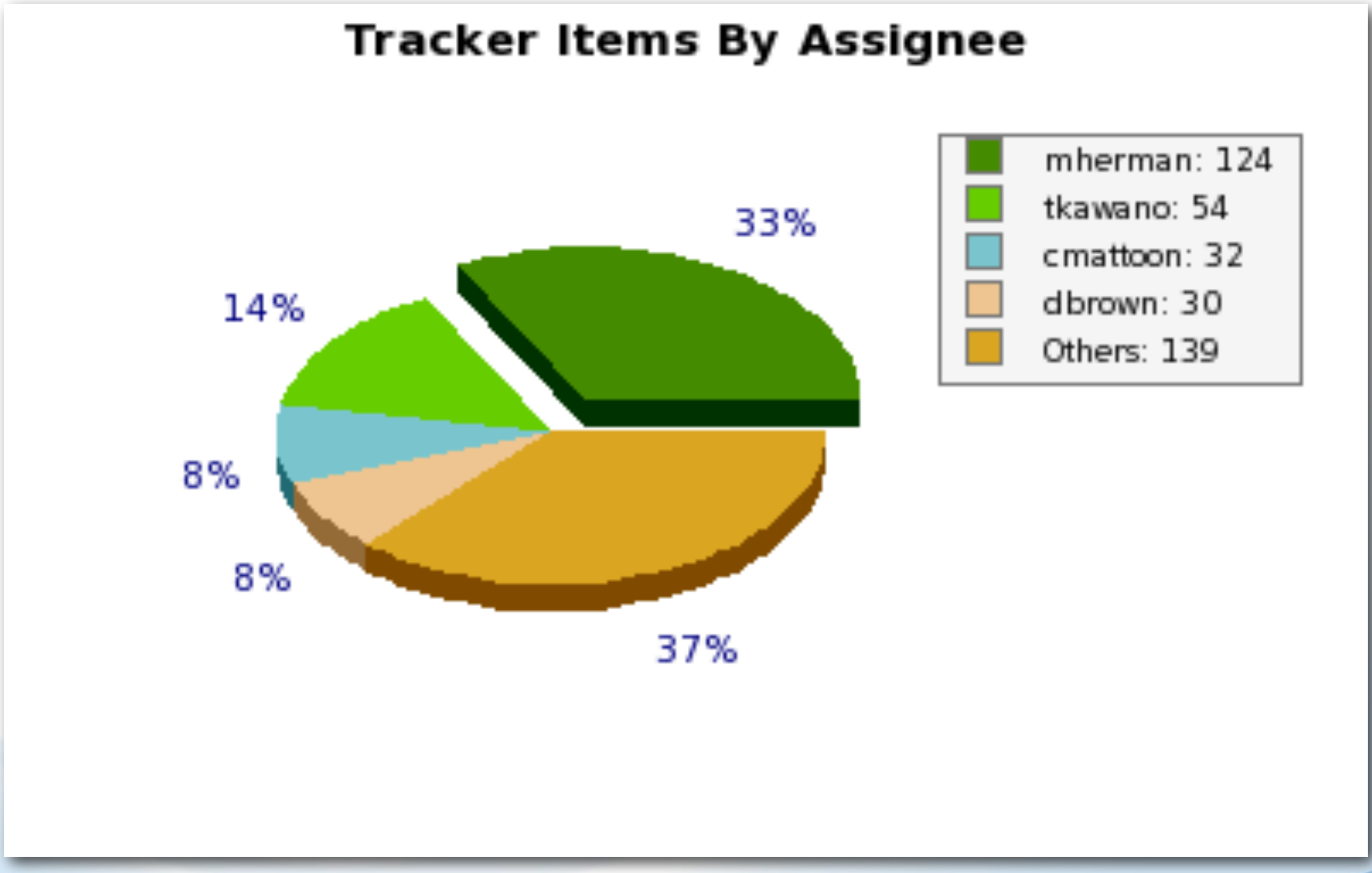
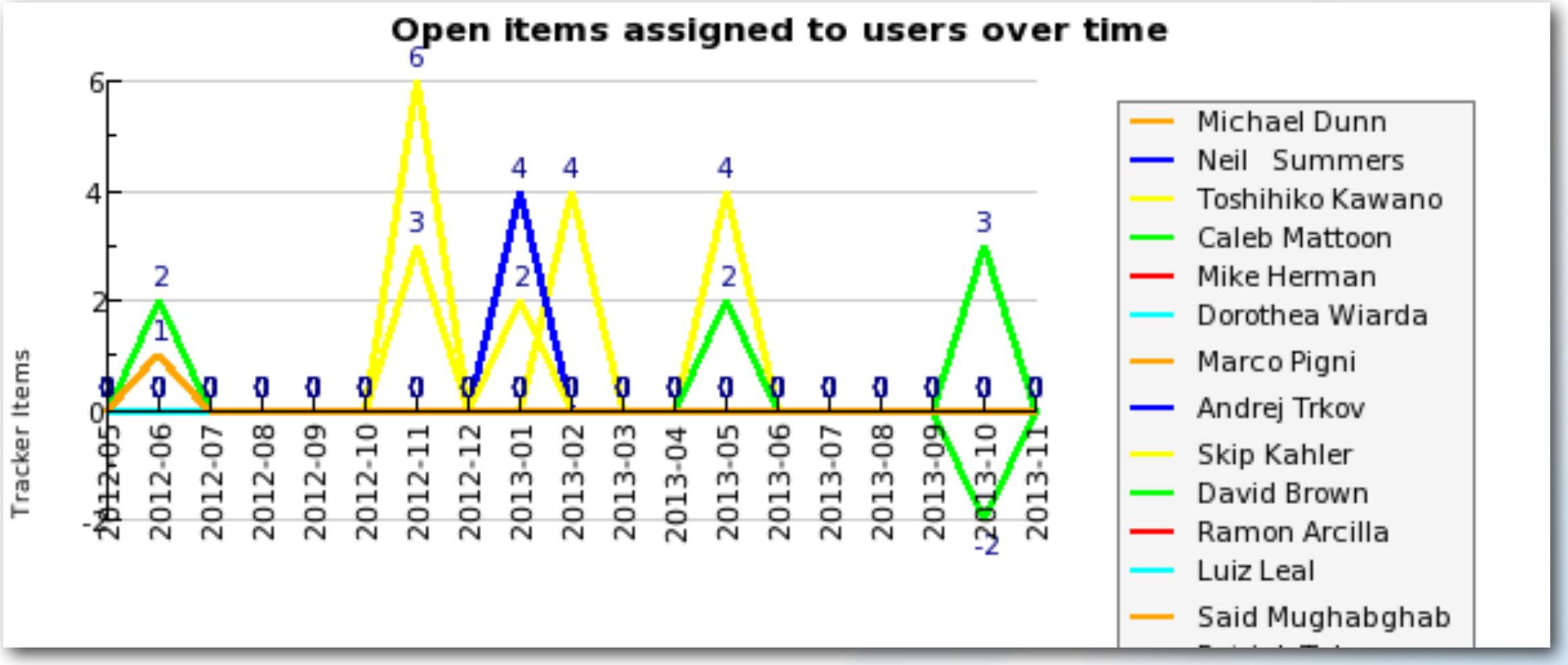
Getting through these and fixing the easy ones will take ~ 2 weeks

Who is submitting the bug reports?



Who is fixing the bugs?



Outline

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- **ENDF/B-VIII**
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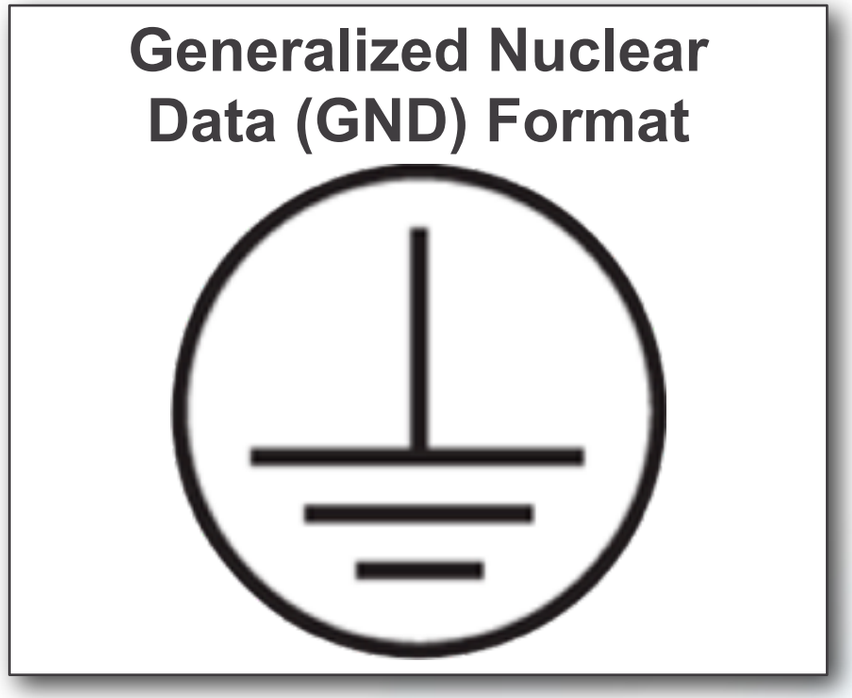
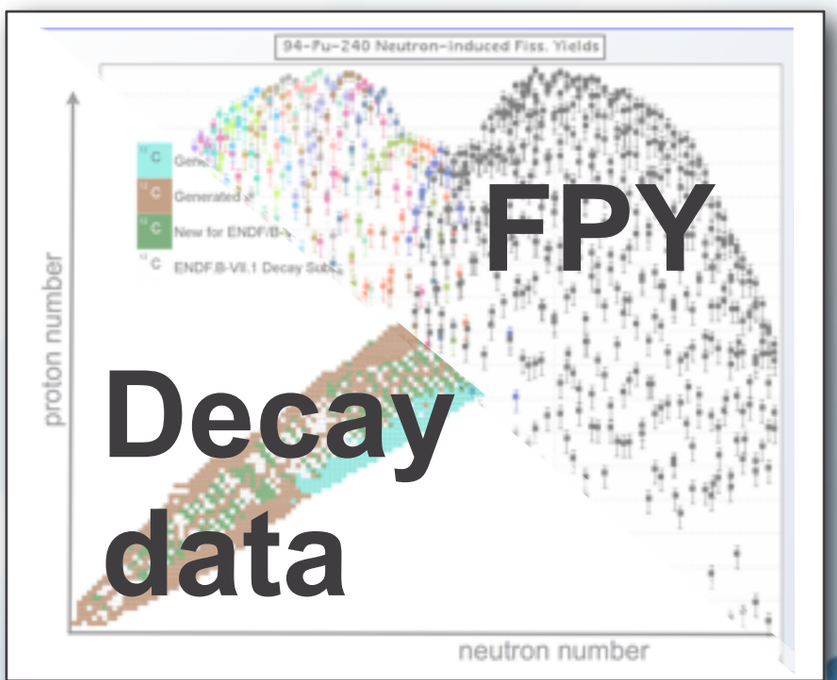
ENDF/B-VIII


CIELO: world-wide reaction data file
Join our CIELO collaboration


Generalized Nuclear Data (GND) Format


Quality Assurance


94-Pu-240 Neutron-induced Fiss. Yields
proton number
neutron number
FPY
Decay data

ENDF/B-VIII

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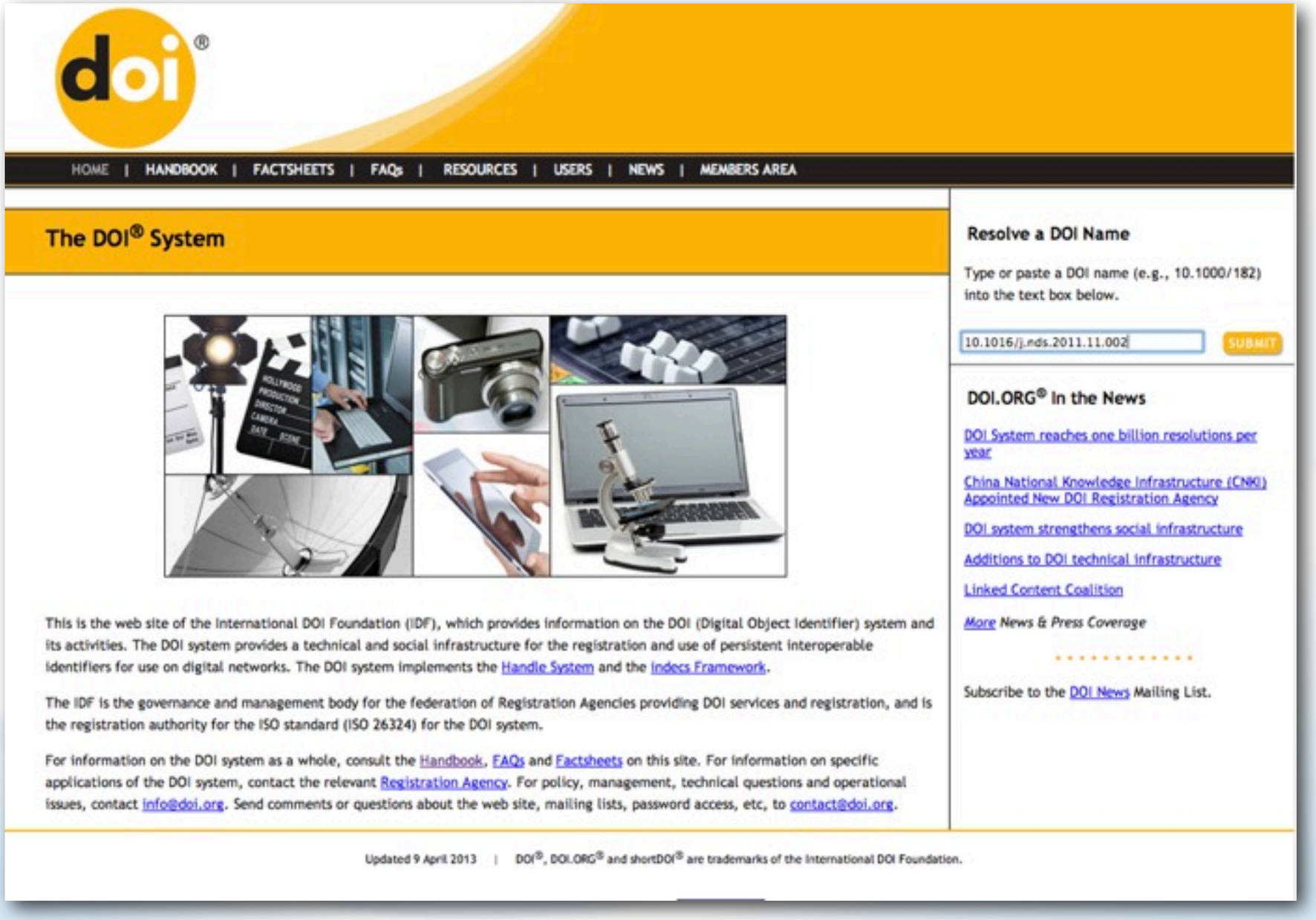

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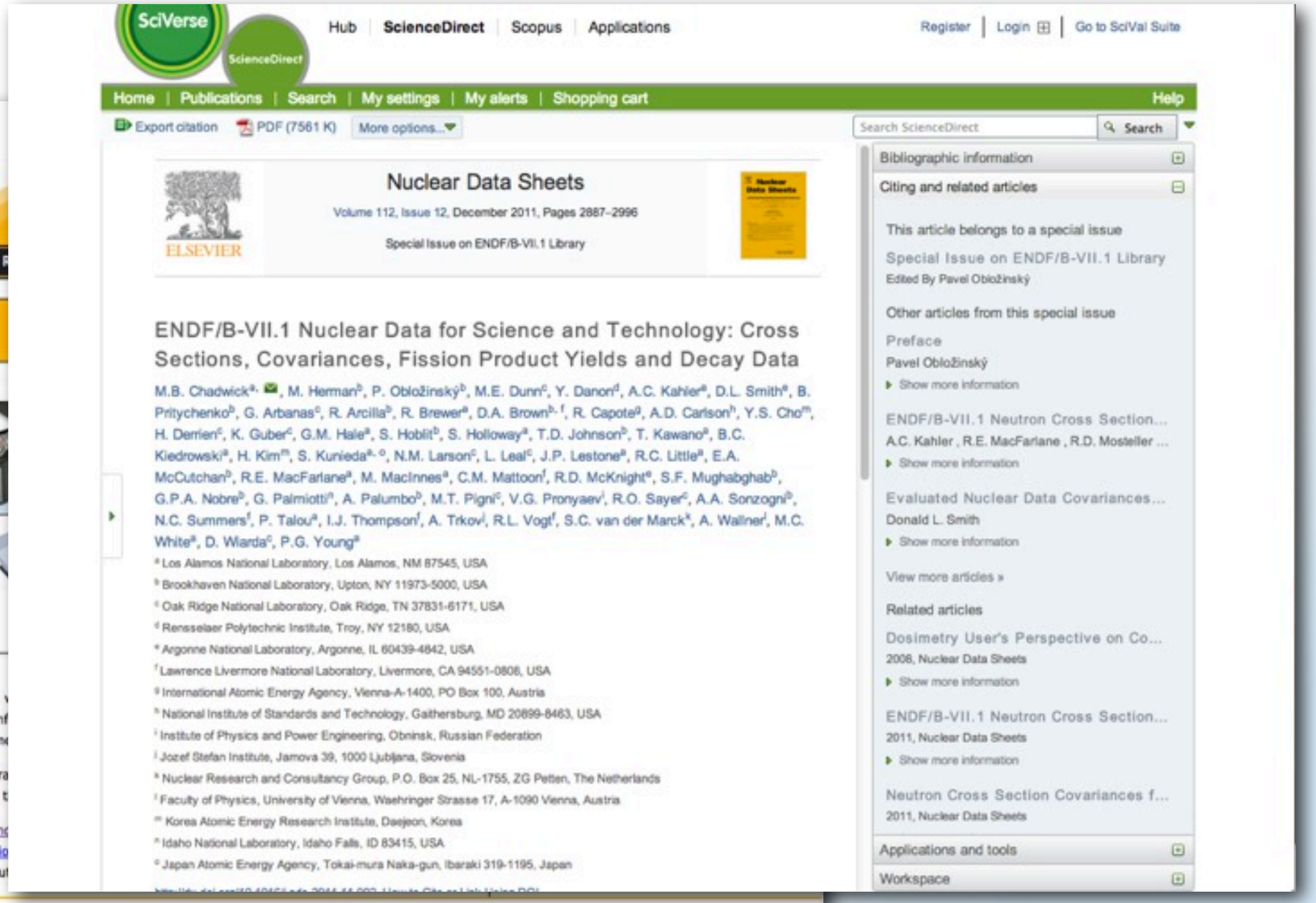
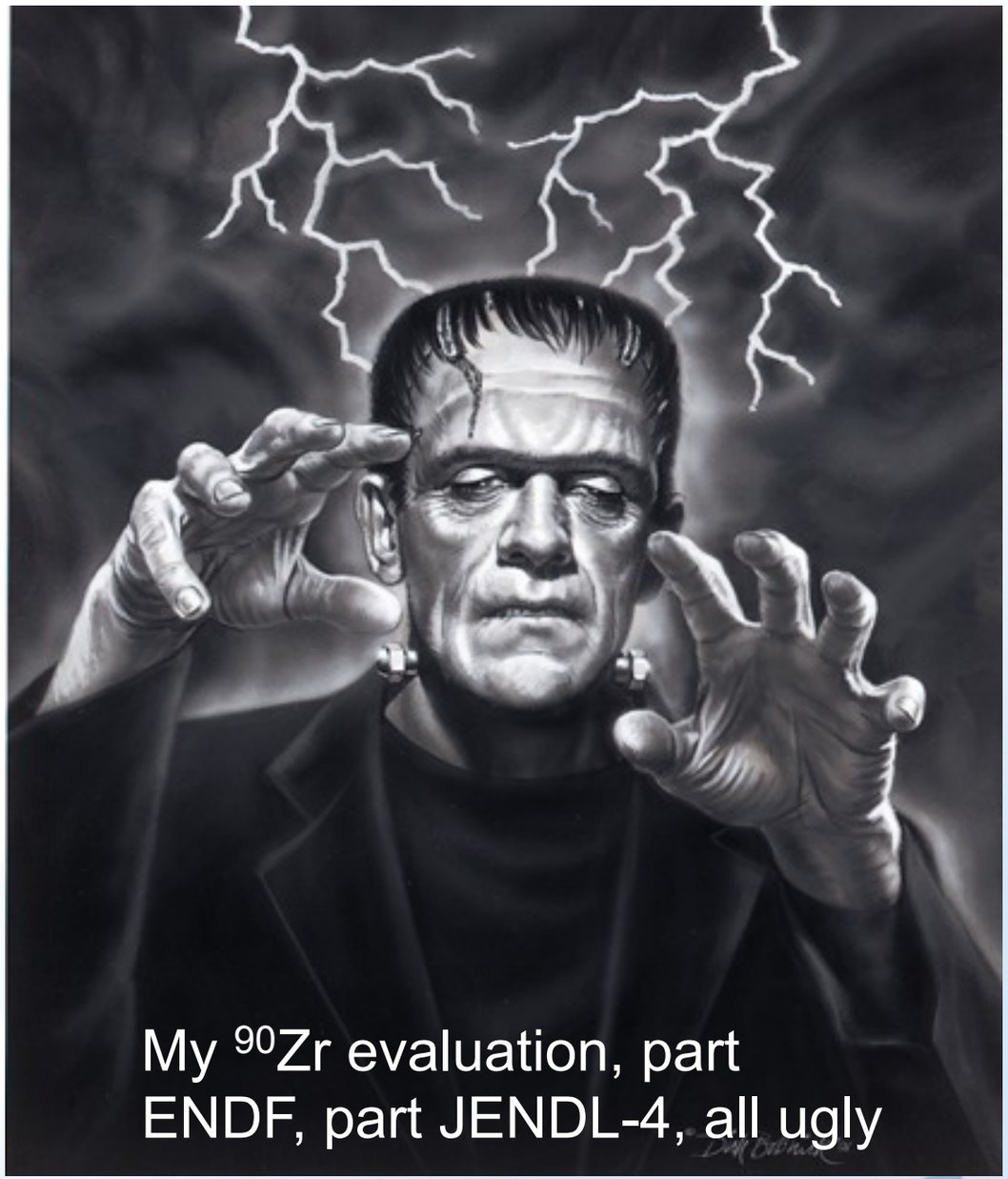


osti.gov and datacite.org want DOI's on all nuclear data in US; likely by end of FY14

- **DOI's are unique id's on a publication/ dataset**
  - NNDC will generate them for NNDC-generated data
  - If CSEWG & USNDP OK, we will assign DOI's for all US nuclear databases
  - We decide on URL scheme
  - We provide a permanent URL to a dataset, datacite.org maintains the DOI->URL redirect
  - We promise to maintain URL's forever (or provide tombstone)
- **This is a very good thing**
  - Gives proper credit to evaluators
  - Generates citations (always good for performance appraisals)

How does this affect us?

- **ENDF borrows from other libraries**
  We'd like to be able to give proper credit; e.g a JAEA DOI for a JENDL-4.0 derived evaluation rather than an NNDC DOI
- **What about partial evaluations?**
  Fine grained DOI's (i.e. on evaluation parts) allow us to make Frankenevaluations with proper attribution.



For ENDF/B series libraries, these are my first thoughts

- **For legacy libraries (ENDF/B-I through VI)**
  - These were distributed in tapes (real or virtual)
  - Each tape provided updates to your center's copy of the library
  - MAT's, MT's and MF's all jumbled
  - Records of what is on what tape and when they were released not easily recoverable
  - Released data != what we see on web
  - **Proposed solution:** One DOI for each release of a library

- **For ENDF/B-VII series**
  - Distinct sublibraries and distinct evaluations
  - One material, zero or one projectile
  - Clear release procedures
  - ENDF format does have clear structure, so could give DOI's for each MF/MT, but we can't tell who evaluated which part
  - **Proposed solution:**
    - One DOI for each evaluation
    - Need DOI's from other centers?

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ENDF Project Pages

- **Reorganized the set of ENDF web pages:** http://www.nndc.bnl.gov/endf/project.html
- **Compiling ENDF history back to ENDF/B-I**
  - Data files
  - Lab reports (BNL & others)
  - Formats
- **Links to ENDF development pages**
- **ENDF QA Page:** http://www.nndc.bnl.gov/endf/b7.dev/qa.html
  - Includes ADVANCE requirements document
  - Various ENDF QA requirements documents