# XML Session Overview

David Brown

Monday 11/14/11
XML Format Session Agenda

- Why a "new" nuclear data format   (Bret, 10 min.)
- Its history
- Why a new "format"   (Mike, 15 min)
- Overview of new format (GND)   (Caleb, 30 min.)
- Associated infrastructure (FUDGE)   (Bret, 10 min.)
- Uses of FUDGE and GND for ENDF/B-VII.1   (Dave, 15 min.)
- Discussion and break   (30 min.)
- Bret's rant!   (Bret, 10 min.)
- Nuclear structure database   (Nidhi, 15 min.)
- Future plans   (Caleb, 10 min)
- Final discussion   (20 min.)
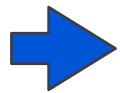
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Summary of session

- Why a new format?
  - Insert punchcard joke here [All]
  - ENDF limitations [B. Beck, M. Herman]
  - Crucial for future of community [M. Herman, others]
- What is GND? [C. Mattoon, B. Beck]
- What is FUDGE? [C. Mattoon, B. Beck, D. Brown]
- What Next?
  - Structure databases [N. Patel, T. Johnson]
  - What FUDGE/GND needs [C. Mattoon, B. Beck]
    - Formats/capabilities
    - Documentation (esp. design philosophy)
  - Adoption/Form a WPEC [R. Forrest]

ENDF-6 format

Will we continue to be enslaved by this "modern technology"?
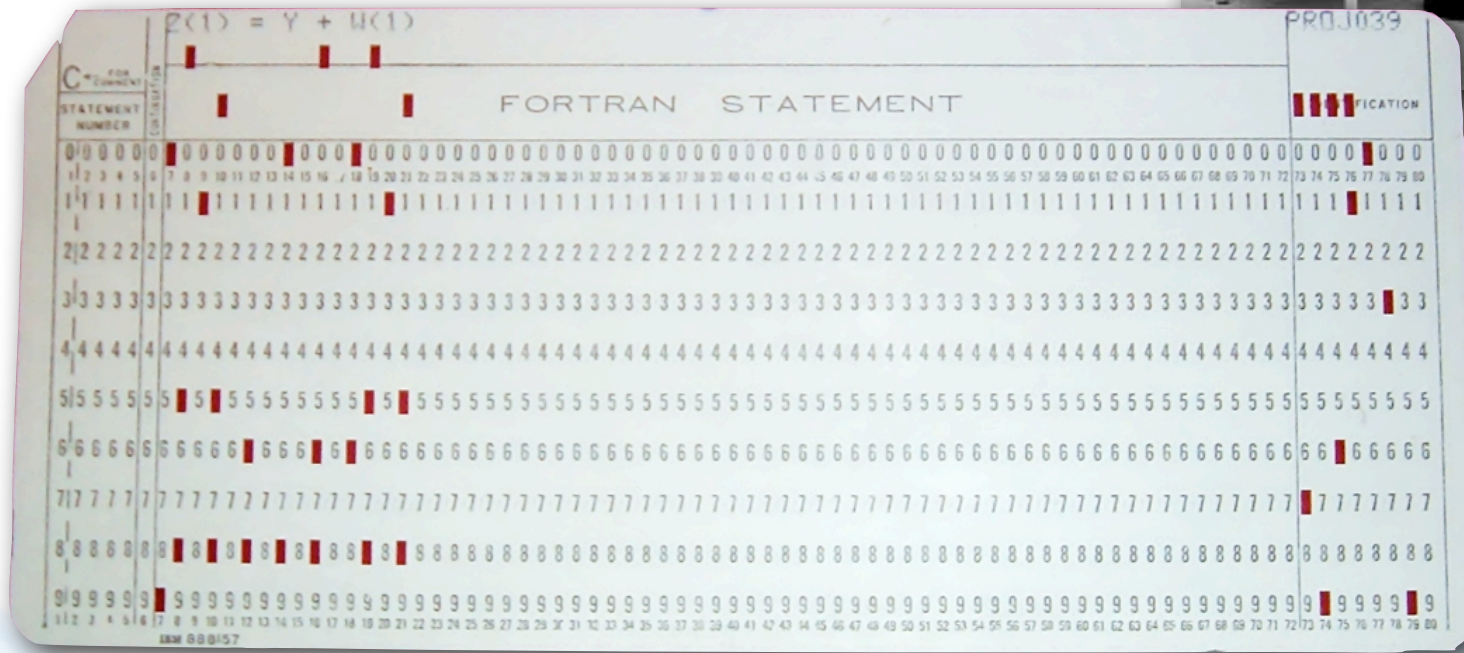
Unfixable problems in ENDF-6

- Rigid structure not lending itself for easy extensions
- Whatever is not in the format can't be stored (processing codes would crash!)
- Fixed number of digits (problem with covariances)
- Dropping 'E' in the exponent is not well received by modern languages
- **Impossible to read by an average homo sapiens**
- Complex coding needed to read, no standard software support
- Does not integrate with other libraries (EXFOR, ENSDF)

Why a new format?

- If we don't think to have ENDF/B-VIII, JEFF-4, JENDL-5,... let's keep ENDF-6 format!

  However,

- If we want to attract skillful(!) adepts we can't ask them to punch holes in the paper (even virtually)
- If we are serious about covariances we need huge data storage with fast access (e.g., HDF5)
- If we want that ND databases evolve we need flexible format, with native software support, so that we do not need spend weeks to implement each format extension
- **Finally, lot of work has already been done with GND!**

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The GND Format

- **The goal:** make one unified structure for all forms of nuclear data: evaluated, MC, deterministic and experimental

- New data hierarchy must be easily human-readable, and representative of underlying physics

- Define a structure, xml is one implementation

Latest version of GND now available to CSEWG on GForge and on the Green Data Oasis:

https://ndclx4.bnl.gov/gf/project/gnd

ftp gdo-nuclear.ucllnl.org

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Format highlights

- Top level GND elements:
  - \<reactionSuite\>
  - \<covarianceSuite\>
- Multiple data forms in one file
  - nativeData attribute tells you what evaluator meant
  - cross section forms:
    - \<backgroundWithResonances\>
    - \<pointwise\>
    - \<grouped\>

- Data stored in hierarchy that mirrors physics
- xData:
  - generalized data containers for GND
  - 2D objects are accelerated w/ C
  - matrices are accelerated w/ numpy
- xLink'ing associates data elements
- xml schema

XML Schema for GND

- Defines the structure of a GND file, and may be used to validate that GND files are properly formatted

- Validation is simple, may be done using online schema:
  - `>xmllint –schema http://.../gnd.xsd gnd_sample.xml`

- Validating catches many format errors:
  - Missing elements or attributes
  - Extra, unrecognized elements or attributes
  - Invalid data in text fields:
    - `<data>1.0e-5 3.8e+3 2.5e-2 2.3 e+3 ...</data>`
  - Incorrect type in attributes (missing units, etc)

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What FUDGE provides

ENDL

ENDF

HDF5

**GND
(XML)**

NDI

ACE

ndf

mcf

tdf
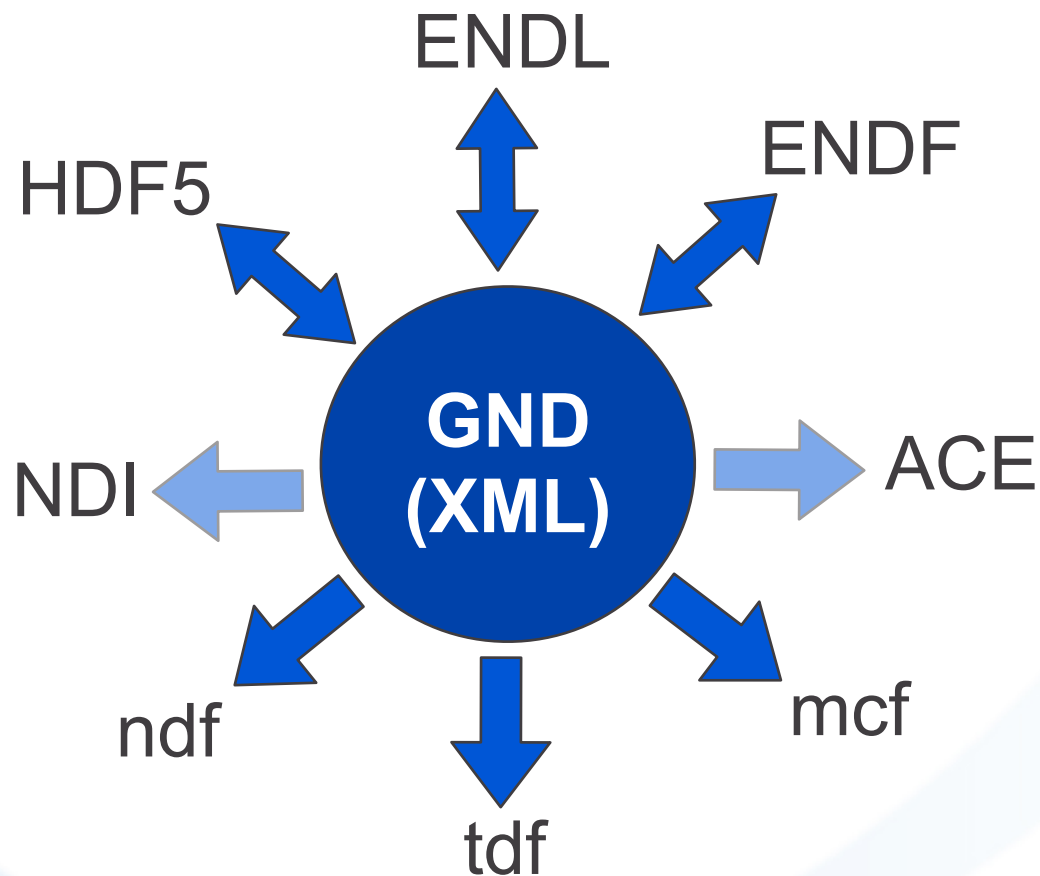
energy deposition/
kermas

common data fixes

data checks

translation

grouping

heating

visualization

resonance
reconstruction

sampling from
covariances

Essentially
one-to-one

Some info.
loss

Planned

12

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FUDGE has matplotlib & gnuplot based plotting and can reconstruct resonances

^{35}Cl(n,g), uses LRF=7

Legend (from plot):
- /Users/davidbrown/Projects/Current/checkendf.trunk/endfb7.1/neutrons/n-017_Cl_035.endf: (n,g)
- (2002) K.H.Guber, L.C.Leal, et al.
- (2004) G.L.Molnar, Zs.Revay, et al.
- (1997) L.Venturini, B.R.S.Pecequilo
- (1969) G.H.E.Sims, D.G.Juhnke
- (1969) G.H.E.Sims, D.G.Juhnke
- (1966) J.H.Gillette
- (1961) R.W.Durham, F.Girardi

Axes: Cross Section (barn) vs E_n (eV)
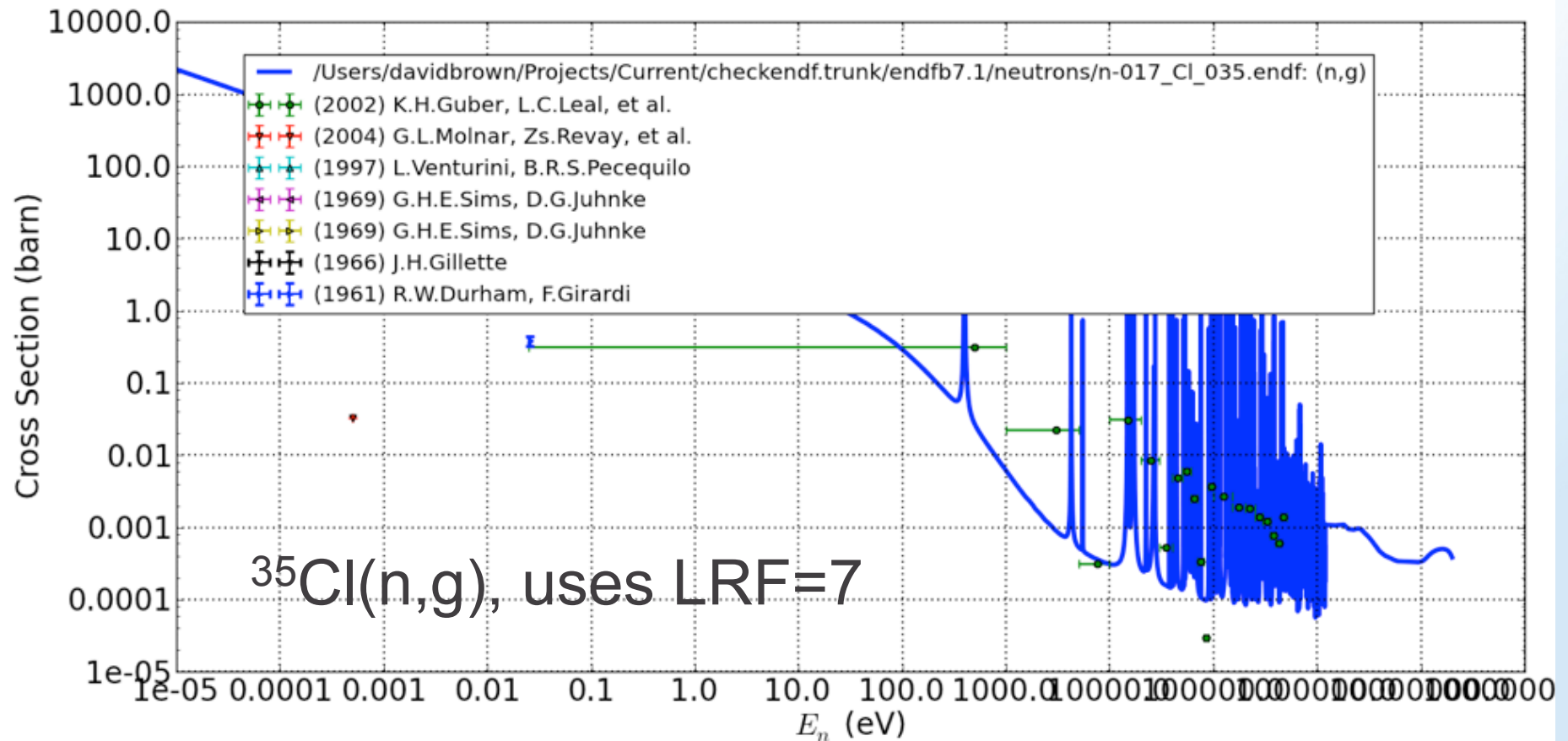
And it can handle covariances
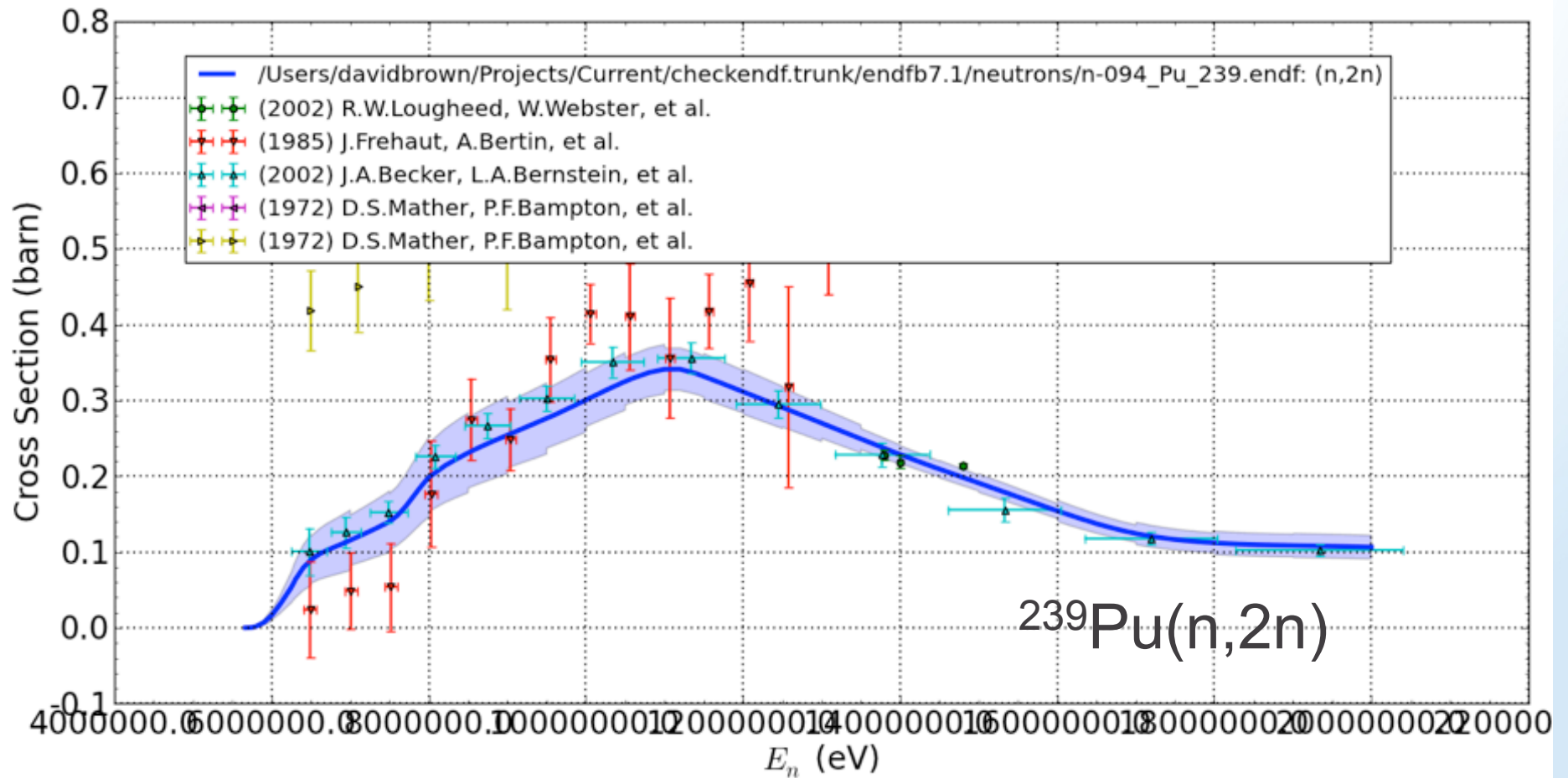
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Some discussion about an XML-based structure format

- N. Patel
  - Extension to RIPL + Audi-Wapstra
  - Geared to reaction data

- T. Johnson
  - First pass at ENSDF replacement
  - See USNDP structure session

- Much more discussion needed to iron out
  - Common needs of structure + reaction communities
  - Common format elements of two communities

To Do list for GND and FUDGE

- **Usability issues**
  - Documentation
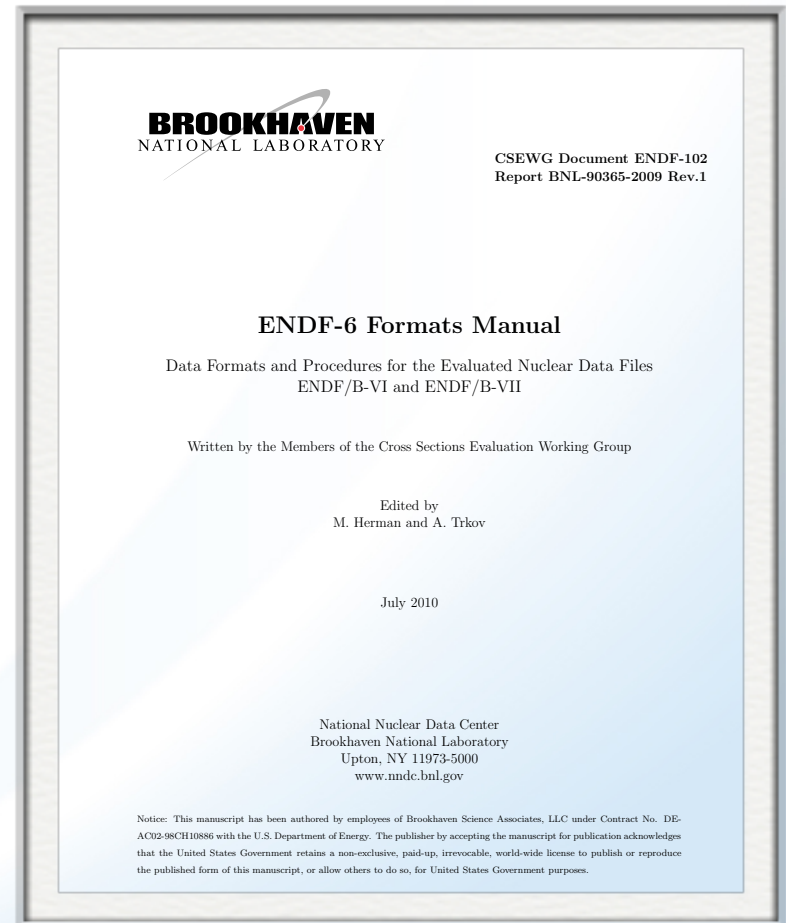 - Design philosophies
  - Python 2 vs. 3
  - numpy dependence
  - C/C++/FORTRAN extensions -- get rid of FORTRAN
- **To do:**
  - Evaluator toolkit/HF code hooks
  - Transport code API: GIDI, being implemented at LLNL, Geant
  - Improved checking, fixing and visualisation
  - ENDF Format loose ends:
    - thermal neutron scattering
    - decay data
    - atomic data
    - misc. minor formats

What needs to be done to encourage international adoption

- CSEWG/USNDP participation in project(s)
  - GForge project page
  - Feedback
  - These are open source projects (format, codes, all of it)
  - Ownership issues
- International participation in project(s)
  - WPEC formation, D. McNabb + CSEWG Formats Committee to propose one
  - get community involved early so they get ownership

What else needs to be done?

- Checking codes - all to be rewritten

- ENDF-6 manual to be updated

- NJOY, AMPEX, PUFF, PREPRO - need new interface

- Web retrieval codes - need new interface

- MCNP and other transport codes essentially not affected

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CSEWG Document ENDF-102
Report BNL-90365-2009 Rev.1

ENDF-6 Formats Manual

Data Formats and Procedures for the Evaluated Nuclear Data Files
ENDF/B-VI and ENDF/B-VII

Written by the Members of the Cross Sections Evaluation Working Group

Edited by
M. Herman and A. Trkov

July 2010

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Feedback wanted

Please download latest FUDGE and check out GND structure!

We need to have good design by March 2012 so we can test access routine for user codes.

Slide from B. Beck

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