Status Report on GND Format Development

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Outline

- Quick review of GND
  - Format versus structure
- What is the purpose of a reaction database?
- Other reasons for a new database “structure”
- Some thoughts on a new reaction database structure

The opinions expressed here are those of Bret Beck and do not represent punchcards

New reaction database

- LLNL has developed a new reaction structure called GND
  - Replaces LLNL's ENDL and ENDF
  - Physics base structure
  - We also provide an infrastructure
    - Data reading/writing
    - ENDF $\Leftrightarrow$ GND
    - Processing: e.g.,
      - deterministic transfer matrix calculation
      - Resonance reconstruction
    - Checker codes (may be the best available)
    - Access routines for transport codes
  - Article to appear in Nuclear Data Sheets
    - See article reasons for new structure
  - Latest release is available with infrastructure at https://ndclx4.bnl.gov/gf/project/gnd

- WPEC subgroup 38 has been set up to design an international structure

For simplicity I will call structure to be developed by WPEC sub-group 38 GND

LLNL's GND defines a structure

- Structure + Meta-language = format
  - GND/XML, GND/HDF5, GND/Python, …
- Basic components of the GND structure are (XML-ish like)
  - Element
  - Dataset
  - Metadata/attributes
    - XML and HDF5 support this directly
    - JSON (JavaScript Object Notation)
      - Only has A and dataset

GND	Element	Dataset	Metadata
XML	Element	Text	Attribute
HDF5	Group	Dataset	Attribute
JSON	Object	Array	Object named 'attribute'
File system	Directory	File	File named 'attribute'

Purpose of reaction database

- What I learned today?
  - Sharing
  - In particular, the purpose of ENDF and a new database structure is for sharing data
    - Less restrictive on size and access time then transport codes
  - What type of data do we want to share
    - Evaluated
    - Processed (Monte Carlo and deterministic)

LLNL's GND allows for simultaneous storage of evaluated and processed data so we can exchange data with others

Other reasons for GND

- Future generations are going to want modern computer practices
  - Make change before next asteroid hits
- Reading legacy Fortran codes can be very difficult
  - Memory tricks
  - FUDGE checking versus ENDF checker codes
- Documentation
  - Hyper links

Some thoughts for WPEC sub-group 38

Thought 1:
Must we rush?

Time line of new structure

- I expect 3-5 years before first release
  - Another reason to start new structure now before asteroid hits
  - LLNL will use its GND and infrastructure during this interval
  - Transition to new structure will most likely be easy

- ENDF to be around at least 10 years
  - ENDF $\Leftrightarrow$ GND
  - although it may not be able to handle all reactions in new evaluations which concerns some but not me

This time line should be considered with the next slide

Computational limits: then, now, tomorrow

Era	Computer	Speed[1] (MIPS)	RAM[1] (MBs)	Disk[1] (GBs)
Early 1980's PC	LSI 11	? (< 0.5)	0.064	0.001 0.02
Early 1980's main frame	VAX 11/780	0.5	2 (8 Max)	0.6
Today	PC	30,000/core	10,000	1,000
5 years	PC	135,000/core	50,000	10,000
10 years	PC	~∞	~∞	~∞

[1] If cost were included, future numbers would be even more favorable.
[2]Okay maybe not quite ∞.

I do not think we should be obsessed with the size of the database

Thought 2:
Must we evolve?

Reactions needed at LLNL

- Reaction in LLNL's ENDL that are not supported by ENDF
  - (z, 2p α):
    - e.g., n + Ni56 -> 2 H1 + He4 + Cr51
  - (z, n p) versus (z, p n) :
    - MT 28 is the sum (z, n p) + (z, p n)
    - e.g.,
      - H3 + He3 $\rightarrow$ H1 + (He5 $\rightarrow$ n + He4)
      - H3 + He3 $\rightarrow$ n + (Li5 $\rightarrow$ H1 + He4)

- NIF may want C12 as a projectile

- Above are not supported by ENDF

This may force transport codes to be particle and reaction blind (i.e., data driven).

Coherent gamma scattering with polarization

- Rayleigh (atomic), nuclear Thomson and Delbrück scattering
- Must add amplitudes not cross sections

$$\begin{aligned}\frac{d\sigma_{\rm p}}{d\Omega} &= (1 + p_{\rm i}\, S_{1{\rm i}} S_{1{\rm f}}) \left(|A_{\parallel}|^2 + |A_{\perp}|^2\right)/4 \\ &+ (p_{\rm i}\, S_{1{\rm i}} + S_{1{\rm f}}) \left(|A_{\parallel}|^2 - |A_{\perp}|^2\right)/4 \\ &+ p_{\rm i}\, (S_{2{\rm i}} S_{2{\rm f}} + S_{3{\rm i}} S_{3{\rm f}}) \left(A_{\parallel} A_{\perp}^* + A_{\parallel}^* A_{\perp}\right)/4 \\ &+ i\, p_{\rm i}\, (S_{2{\rm i}} S_{3{\rm f}} - S_{3{\rm i}} S_{2{\rm f}}) \left(A_{\parallel} A_{\perp}^* - A_{\parallel}^* A_{\perp}\right)/4\end{aligned}$$

Stokes parameter

There should be no restriction on projectile, target or reaction

Correlations in outgoing products are being requested

- Currently, many evaluations (or reactions) allow for the “right” answer on average

- More and more, at LLNL we are required to get the answer right event by event
  - For many reactions, this may only be solved with a model but GND should not limit correlated data where possible

Thought 3:
Must we lose?

Deprecating some ENDF distribution types

- We should consider removing some ENDF type for future evaluations

- MF = 5
  - Examples: Evaporation and models

Just a thought!

Thought 4:
Must we split?

Other possible databases

- How do I view GND?
  - As a nuclear reaction database
  - ENDF has sub libraries which, in part, I view as different databases

- Particles
  - Mass, halflife, nuclear levels, atomic levels, …
  - Required
  - Linked to by nuclear reaction database
- Physical constants
  - Would be nice

- Others?

- All database may share data types

Thought 5:
Must we hobnob?

Wiki: pronounced ‘We Key’

- For WPEC sub-group 38 I think we should set up something like a wiki
- Should have an outline of the current design
- Anybody can comment
- Where can this be set up so that a password is not required; or should it be?

We key to a good structure;
need input/feedback from community

Summary

- Things to consider for WPEC sub group 38
  - Reaction database versus other databases?
  - For reaction database; evaluated and processed data?

- Thoughts
  - Memory and speed should not be an issue
  - New reactions and data types should be allowed
  - Deprecate some data types?
  - Splitting database
  - Wiki - we key

- Structure/Format is not enough
    - Checker codes
    - Processing codes
    - New evaluation V&V (e.g., testing)
- ENDF $\Leftrightarrow$ GND

  - New evaluations
    - may have reactions not supported by ENDF (oh well)
    - LLNL wants more complete product list (n, H1, H2, H3, He3, He4 and γ)