Some thoughts on the structure to replace the ENDF-6 format

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LLNL-PRES-??????

I will use the new reaction structure GND as an example

- LLNL has developed a new nuclear reaction database
  - Called GND
  - Has supporting infrastructure
  - Latest release is available with infrastructure at https://ndclx4.bnl.gov/gf/project/gnd

Divide ENDF into reaction and particle databases to reduce redundancy and to add clarity.

- I see ENDF as a collection of several databases
  - Reaction and particle database, and maybe others

- Divide into several databases
  - Nuclear reaction database

    $n + O16 \rightarrow n + p + N16$

    $n + O16 \rightarrow n + O16\_e3$

  - Other needed databases
    - Separate data common to multiple reaction databases into other databases
    - Examples
      - Particle database: Name, mass, spin, levels, etc.
        - » Decay: independent of history (e.g., input channel)
      - Physical constants
      - Others?

Within a database put common information together to reduce redundancy and to add clarity

- GND as an example
  - Structure
    - Documentations
      - ENDF, html/XML with links, from processing codes
    - Data common to multiple output channels
      - Particle list (all particle information here)
      - Resonance data (already in one place in ENDF)
    - Reaction (one for each unique output channel)
    - Summed data (e.g., total cross section)

ENDF/B-VII.1 Am242m1 error becomes clearer when like data are collected together as is done in GND.

```
<particle name="Am242" genre="nucleus" mass="242.059455171546 amu">
    <level name="Am242_e0" label="0" energy="0 eV"/>
    <level name="Am242_e1" label="1" energy="48600 eV" spin="5"/>
    <level name="Am242_e2" label="2" energy="44100.002 eV"/>
    <level name="Am242_e3" label="3" energy="52900.002 eV"/>
      ...
```

Design should not restrict allowed reactions.

- (z, n p) versus (z, p n) :
  - MT 28 is the sum (z, n p) + (z, p n)
  - e.g.,
    - H3 + He3 → H1 + (He5 → n + He4)
    - H3 + He3 → n + (Li5 → H1 + He4)
    - H3 + He3 → n + H1 + He4
- In GND we added ”process” qualifier to separate some reactions.
  - Example: shape and compound elastic

- reaction outputChannel=“n + O16 → n + O16” process=“shape”
  - crossSection
  - outputChannel
    - n
    - O16
- reaction outputChannel=“n + O16 → n + O16” process=“compound”
  - crossSection
  - outputChannel
    - n
    - O16

Li6 + Be9 → (Li6_e2 → H2 + He4) + (Be9_e1 → n + He4 + He4)

Use nested structure to clarify flow.

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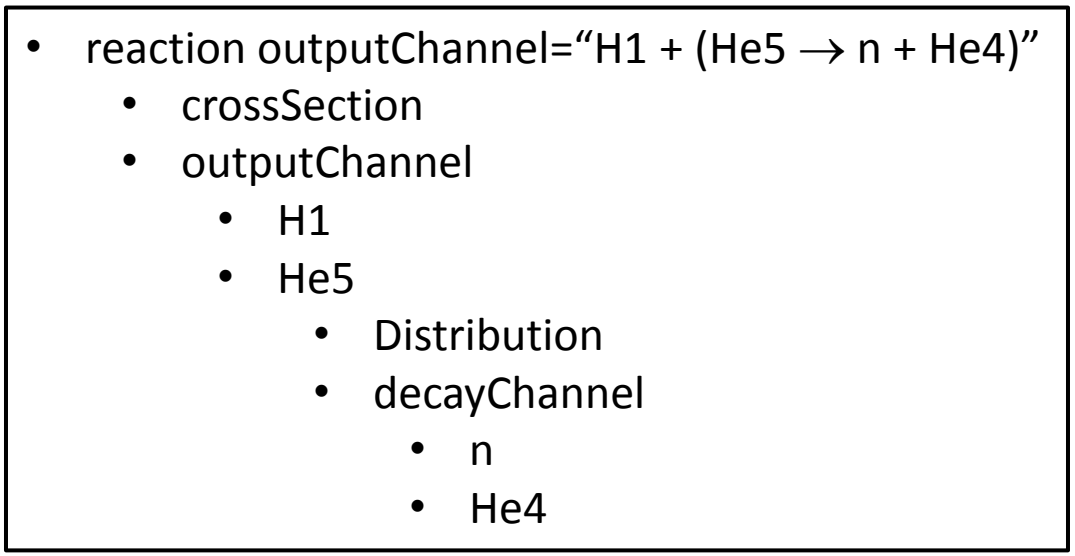
    - H3 + He3 → n + (Li5 → H1 + He4)
    - H3 + He3 → n + H1 + He4
- GND nest decayChannel within its parent: example



Any product can have a decay channel.

The finer the reactions are resolved the more checking possible between evaluations

- An important asset of ENDF is the sharing and comparing of evaluations.
  - ENDF limits detailed comparisons by limiting reaction types and forms for the data
- Unlimited reactions discussed in prior slide
- It would be nice to add processed data to the sharing and comparing
  - GND supports this by allowing various forms of a dataset to be stored
  - GND allows simultaneously storage of the different forms
  - Example:
    - Cross section
      - Resonances with background (original data)
      - Pointwise (derived data)
      - Grouped (derived data, use for deterministic transport)

Interpreting and other codes shall be driven by data

- Processing codes must not make any assumes about how to handle the data.
  - ENDF example from Kalbach/Mann data.
    - f(E,E')
    - r(E,E')
    - a(E,E')

    } These all share the same interpolation flag.

    - Better to have interpolation flag for each as in general it is better to use unit-base interpolation for f(E,E') and not for r(E,E') and a(E,E').

Summary

- Divide ENDF into reaction and particle databases to reduce redundancy and to add clarity
- Within a database put common information together to reduce redundancy and to add clarity
- Design should not restrict allowed reactions
- Use nested structure to clarify flow
- The finer the reactions are resolved the more checking possible between evaluation
- Interpreting and other codes shall be driven by data

More on GND

- 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 element 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’

Too much nesting can also be a problem

- Two difference ways to store pointwise cross section data

GND currently

```
<data>
   17882500 0
   1.8e7       0
   1.9e7       0.0441259
   2e7          0.207599
</data>
```

More nesting

```
<data>
   <xy> <x> 1.78825e7</x> <y> 0</y> </xy>
   <xy> <x> 1.8e7</x>       <y> 0</y> </xy>
   <xy> <x> 1.9e7</x>       <y> 0.0441259</y> </xy>
   <xy> <x> 2e7</x>         <y> 0.207599</y> </xy>
</data>
```

Surprisingly, the more nesting could take much more memory in binary form. HDF5 groups are like directories, they consume space even when empty!

Avoiding duplicity

- For GND we tried to eliminate duplicity.
  - Example, the mass of each particle is only stored once.
- Currently in GND for a pointwise cross section we store its length and its data.
  - Some do not want the 'length' attribute.
  - Length is number of {x,y} pairs.
    - Advantage: Access routine know how much memory to allocate.
    - Disadvantage: Syncing with data (by manual editing for example).
- Example: Cross section
  - Length

    <linear xData="XYs" length="132" accuracy="0.001">
  - Data

    1e-5 1.6649 1 1.6649 … 2e7 0.60581

- For other data, like $P(\mu|E)$, GND does not store the length for the number of E's but for a given E_i its $P_i(\mu)$ does list the number of $\{\mu_j, P_{i,j}(\mu_j)\}$ pairs.

Avoiding duplicity: Another issue with GND

- In GND, each dataset has “axes” information
  - Label, unit, interpolation and frame
  - Example for a cross section:

```
<axes>
      <axis index="0" label="energy_in" unit="eV" interpolation="lin,lin" frame="lab"/>
      <axis index="1" label="crossSection" unit="b" frame="lab"/>
</axes>
```

- It would probably be better to have axes templates which are referenced with ability to override attributes.

```
<axes ref=“crossSectionAxes”>
      <axis index="0” interpolation=”log,lin”/>
</axes>
```

In ENDF, all axes information but interpolation are implied. GND makes it explicit. This is also something to consider.

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 ∞.

Other possible data needed

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

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

Stokes parameter

Amplitude

There should be no restriction on projectile, target or reaction