Update on recent changes to GND (60')

WPEC Subgroup 43, May 15 2017

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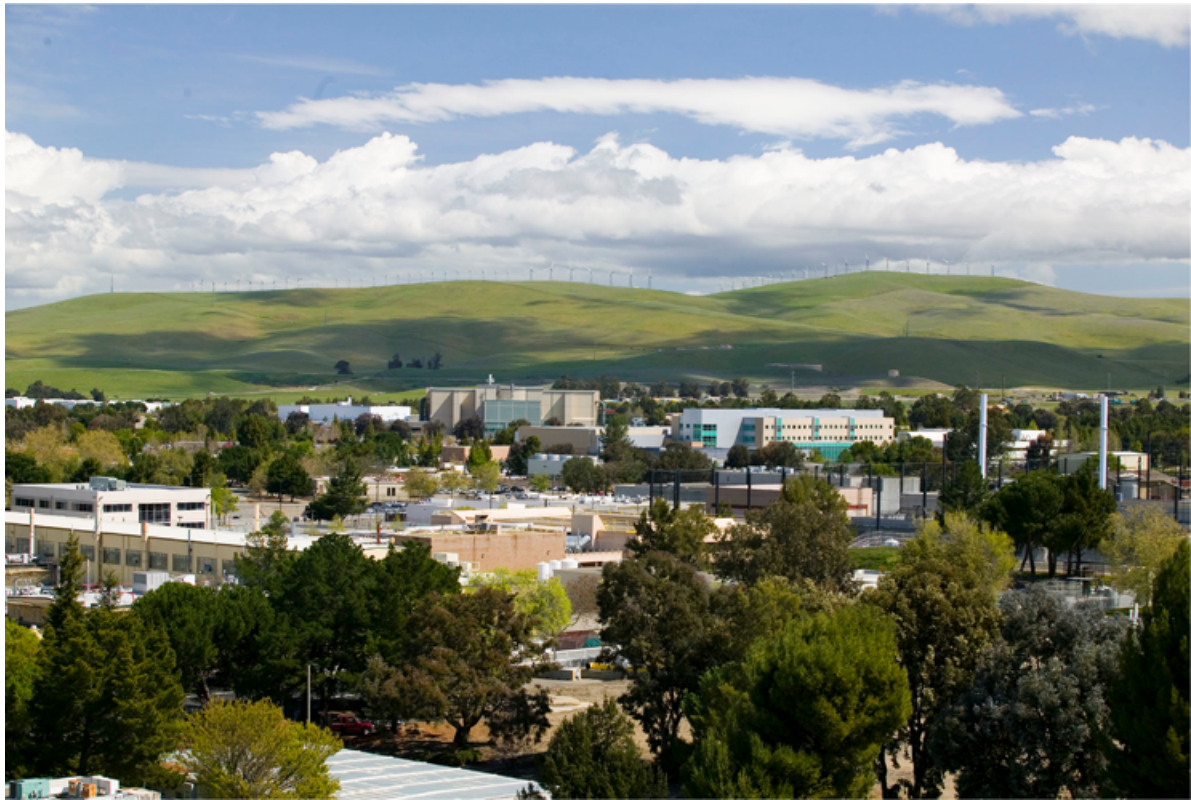

LLNL-PRES-730621

This work was performed under the auspices of the U.S. Department of Energy by Lawrence Livermore National Laboratory under contract DE-AC52-07NA27344. Lawrence Livermore National Security, LLC

Example GND file

- Caleb and I have release GND files for all to view
  - Nearly accurate with SG38 discussions

- GND/XML files for
  - ENDF to GND/XML translation
  - Monte Carlo processed files with 3 cross section temperatures
  - Multi-group deterministic processed files with 3 temperatures
  - Now know how to put Monte Carlo and multi-group deterministic processed files in one file

- If you did not get the email about the release from me, let Caleb or me know

Four requirements/specifications

- PoPs (Property of Particles database)
- Low level data and function containers
- Top level hierarchy
- Documentation (Ask Dave Brown)

I will focus on what I think are still undecided?
Mostly likely not complete.

PoPs (Property of Particles database)

PoPs (Property of Particles database)

- Default quantity from list.
- <Isotope> and <IsotopeWithExcitedNucleus> elements
- <nucleus> element
- Decay library and fission product yields
- ?

Default quantity from list

- How do we mark the ‘default’ value?
  - Leave ‘label’ blank (not good for xlink)
  - Label attribute must always have value of ‘default’
    - or some other standard value
  - ?

```
<isotope id="O16" A="16">
  <mass>
    <double label="default" value="15.994913988" unit="amu"/>
    <double label=”other" value="15.9949226" unit="amu"/></mass>
  <charge>
    <integer label="default" value="0" unit="e"/></charge>
  <nucleus id="o16_e0" index="0">
    <spin>
      <fraction label="default" value="0" unit="hbar"/></spin>
    <charge>
      <integer label="default" value="8" unit="e"/></charge>
    <energy>
      <double label="default" value="0.0"unit="eV"/></energy>
            </nucleus></isotope>
```

Isotope/IsotopeWithExcitedNucleus

- Currently, we (FUDGE) write the <isotope> element as

```
<isotope id="O16" A="16">
    <nuclearLevel id="O16_e0">
        <mass> … </mass>
            …
        <nucleus id="o16_e0" index="0>
            <energy>
                <double … /></energy></nucleus></nuclearLevel>
    <nuclearLevel id="O16_e1">
        <nucleus id="o16_e1" index="1">
            <energy> … </energy></nucleus></nuclearLevel>
    <nuclearLevel id="O16_e2">
        <nucleus id="o16_e2" index="2"> ... </nuclearLevel><isotope>
```

- SG38 elected at the last meeting to remove id='O16_e0' and only have id='O16'
- How do we do this and have isotopes with nuclear excited levels?

<Isotope>/<IsotopeWithExcitedNucleus>: Example

- As can be seen, I think we need to be clear about what the particle is.

```
<isotope id="O16" A="16">
    <mass> … </mass>
        …
    <nucleus id="o16" index="0>
        <energy>
            <double … /></energy></nucleus>
    <isotopeWithExcitedNucleus id="O16_e1">
        <nucleus id="o16_e1" index="1">
            <energy> … </energy></nucleus></isotopeWithExcitedNucleus>
    <isotopeWithExcitedNucleus id="O16_e2">
        <nucleus id="o16_e2" index="2"> ...
            </isotopeWithExcitedNucleus><isotope>
```

<nucleus> element

- How do we specify the excitation of the nucleus?
- Currently, we make the <nucleus> a particle inside of its <isotope> element

```
<isotope id="O16" A="16">
    <mass> … </mass>
        …
    <nucleus id="o16" index="0>
        <energy>
            <double … /></energy></nucleus><isotope>
```

- In my opinion, this has several advantages
  - Nucleus reside with isotope, clear association
  - Does not confuse atomic and nuclear data
    - E.g., <spin> for nucleus is inside <nucleus>
  - Inherits properties from <isotope> (e.g., ‘base’ mass)
- Dave proposed to have an <ion> element

Decay library and fission product yields

- Need to support decay library
  - Dave, Caleb and I are still working on translating it
  - Need to add outgoing particle spectra
  - In my opinion, the ENDF decay format is a mess!!!

- How to store fission product yields
  - Dave should probably lead this discussion

?

Low level data and function containers

Low level data and function containers

- Length attribute for <values> element
- Array
- Uncertainties
- Tables
- ?

Length attribute for <values> element

- The length attribute

```
<values length="8"> 1.019 8.23 ... 1.024 8.17</values>
```

- Initially, SG38 was in favor of having the ”length” attribute for the <values> element as it
  - allows one to know how much memory to allocate and
  - is a way to check that the proper number of values was written

- Now the opinion seems to have changed

Array

- Caleb should lead this discussion

Uncertainties

- Caleb had a good proposal at the last SG38 meeting. He should lead this discussion

Tables

- Caleb should lead this discussion

?

Top level hierarchy

Top level hierarchy

- <documentation> element
- Orphan products
- Axes templates
- Fission products / delayed neutrons
- ?

<documentation> element

- One question:
  - Should this be at the top or in each ‘style’s element?

Orphan products

- Where to put products that are not associated with a particular reaction
  - This is currently gammas in MT 3 and 4
- Originally, SG38 decided to put them under the <reactions> element
- This, I have discovered, is awkward for codes to use.
  - In MCGIDI, I have a reactions and an orphanProducts member as they need to be treated differently

```
<reactions>
    <reaction>
    <reaction>
    …   </reactions>
<orphanProducts>
    <reaction>
    <reaction>
    …   </ orphanProducts >
```

Orphan products

- I would like something like:

```
<reactions>
        <reaction>
        <reaction>
        …                    </reactions>
<orphanProducts>
        <reaction>
        <reaction>
        …                    </orphanProducts >
```

Axes templates

- We still have not implements axes templates in FUDGE/GND nor do we have a design.
- Currently, every physical quantity has an <axes> element like:

```
<XYs1d label="eval">
    <axes>
        <axis index="1" label="energy_in" unit="eV"/>
        <axis index="0" label="crossSection" unit="b"/></axes>
    <values length="564">
        6.43e+6 0.000 ... 20e7 0.0 </values><XYs1d>
```

Fission products / delayed neutrons

- Current way FUDGE/GND stores fission products

```
<products>
    <product name="n" label="n" emissionMode="prompt">
            … </product>
    <product name="n" label="n__a" emissionMode="delayed”
        decayRate="0.013336 1/s">
     <product name="n" label="n__b" emissionMode="delayed”
        decayRate="0.032739 1/s">
        …            </products>
```

- Somethings I do not like about this
  - No heavy products (gamma are there just not shown).
  - Decay rate associated with delayed neutrons

Fission products / delayed neutrons

- Possible alternative

```
<products>
    <product name="n" label="n">      … </product>
    <product name=”photon" label=”photon”> … </product>
    <product name=”photon" label=”photon__a”> … </product>
                                        </products>
<fissionFragments>
    ... </fissionFragments>
```

- Not sure what is under <fissionFragments> element.
- Delayed neutron would be under < fissionFragments> element.
- Can store fission product yields also

Name changes

- There as been must discussion in the past about what to name the top element.
- LLNL currently calls it <reactionSuite>
  - Yes Dave, you named it that!
- I would like it to the <protare> as this psuedo-acronym represents the contents.
  - ProTare = PROjectile + TARget + Evaluate
    - n-008_O_016.endf for ENDF/B.VII.1 (MAT = 825)
    - p-008_O_016.endf for ENDF/B.VII.1 (MAT = 825)
    - n-008_O_016.endf for ENDF/B.VIII.0 (MAT = 825

<reactionSuite projectile="n" target="U235" evaluation="ENDF/B-7.1" version="GND 1.7" … >

<protare projectile="n" target="U235" evaluation="ENDF/B-7.1" format="1.7" … >

?

Documentation

Date format.

- I think we still need to define the format for date.

?