Particle Database update

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Particle database specification appears to be complete.

- Status of requirements / specifications document
- Actual implementation partly complete (translations of ENDF and RIPL)
- How does particle database integrate with GND?
  - Overriding part of the particle database (if necessary): discussed, not yet implemented
- On a related note… recent proposal made by A. Hurst (LBNL) for modernizing ENSDF
  - Common ground between new ENSDF and the particle database?

Specifications for particle database are fairly stable, only changes since last meeting are to wording.

- Requirements / specifications currently 28 pages
- Some new proposals to consider, would change the specifications:
  - Rather than using <quantity> to store every value (i.e. of mass, charge, halflife, etc.), use more specific tags like <double>, <integer>, <string>, etc.
  - Also change specifications for <uncertainty> to allow more specific names like <variance>, <asymmetricUncertainty>, <covariance>, etc.
  - Goal in both cases is to make the hierarchy more explicit about what type of data it contains, due to feedback from SG38

Quick summary of particle database specifications:

```
<particleDatabase formatVersion=”…" library=”…"
        libraryVersion=”…" date=”…”>
  <documentation> ... </documentation>
  <bibliography> ... </bibliography>
  <aliases> ... </aliases>
  <bosons> ... </bosons>
  <leptons> ... </leptons>
  <chemicalElements> ... </chemicalElements>
</particleDatabase>
```

Quick summary of particle database specifications:

```
<chemicalElement name="Magnesium" Z="12" symbol="Mg”>
  <isotope name="Mg32" A="32”>
    <mass recommended=‘…’>…</mass>
    <nuclearLevels>
     <nuclearLevel id="Mg32_e0" index="0" alias="Mg32”>  <energy/><spin/><parity/><halflife/>
       <decays>
         <decay index="0" mode="betaMinus”>
           <probability>…</probability><Q>…</Q>
           <product pid="Al32"/><product pid="e-"/><product pid="nu_e-_anti"/></decay>
         <decay index="1" mode="betaMinusDelayedNeutron”>
           <probability>…</probability>
           <product pid="Al31"/><product pid="n"/><product pid="e-"/><product pid="nu_e-_anti"/>
         </decay></decays></nuclearLevel>
 ... </nuclearLevels> </isotope> </chemicalElement>
```

Particle database supports multiple assignments (i.e. for particle spins), but one must be the ‘default’ or ‘recommended’ value:

```
<spin recommended=‘quantity[@label="0"]’>
  <quantity label="0" value="1/2" unit="hbar"/>
  <quantity label="1" value="3/2" unit="hbar"/>
  <quantity label="2" value="5/2" unit="hbar"/>
</spin>
```

- If ‘recommended’ not supplied, should it default to 1st one in the list?

Database supports uncertainties:

```
<mass recommended='quantity[@label="atomic"]'>
  <quantity label="atomic" value="54.93804514" unit="amu">
    <uncertainty value="7.3e-7"/></quantity>
  <quantity label="massExcess" value="-57710.58" unit="keV">
    <uncertainty value="0.68"/></quantity>
  <quantity label="bindingEnergyPerNucleon" value="8764.988"
            unit="keV">
    <uncertainty value="1.2e-2"/></quantity>
</mass>
```

- Also supports asymmetric uncertainties (see later slide)

Each particle (including nuclear ground and excited states) gets a unique id. Additional 'qualifier' used to specify *atomic* properties

- Pb208_e1 = Lead-208 in the first excited (nuclear) state
  - Particle assumed to have full complement of 82 electrons

- Missing electrons specified with qualifier:
  - Pb208_e1{e+2} missing two electrons
  - Pb208_e1{1s1/2;2s3/2} missing from specific states

- Qualifiers section of spec. document needs more detail. At least needs to cover cases in the atomic relaxation sub-library

—Possible specification changes

All quantities are currently wrapped in a tag called … <quantity>! Should we be more specific about type of quantity? For example:

Current status:

```
<halflife>
  <quantity label=”measured" value=“23.789" unit=”y">
    <documentation>...</documentation>
    <uncertainty pdf="normal" type="variance" value="1.1e-3"/>
  </quantity></halflife>
```

Or

```
<halflife>
  <quantity label=“observed” value=“stable”/></halflife>
```

New proposal:

```
<halflife><double label=“measured” value=“23.789” unit=“y”>…</double></halflife>
```

Or

```
<halflife><string label=“observed” value=“stable”/></halflife>
```

- Other types of quantity: <integer> and <fraction> (especially for spins)

<mass> element may contain many mass-like quantities: bindingEnergy, neutron separation, etc. Should those be promoted a level?

Rather than:

```
<mass recommended='quantity[@label="atomic"]'>
  <quantity label="atomic" value="54.93804514" unit="amu">…</quantity>
  <quantity label="massExcess" value="-57710.58" unit="keV">…</quantity>
  <quantity label="bindingEnergyPerNucleon" value="8764.988"
        unit="keV">…</quantity>
</mass>
```

New proposal:

<mass>…</mass> or perhaps <atomicMass>…</atomicMass>
<massExcess>…</massExcess>
<bindingEnergyPerNucleon>…</bindingEnergyPerNucleon>

<mass> element may contain many mass-like quantities: bindingEnergy, neutron separation, etc. Should those be promoted a level?

Rather than:

```
<mass recommended='quantity[@label="atomic"]'>
  <quantity label="atomic" value="54.93804514" unit="amu">…</quantity>
  <quantity label="massExcess" value="-57710.58" unit="keV">…</quantity>
  <quantity label="bindingEnergyPerNucleon" value="8764.988"
        unit="keV">…</quantity>
</mass>
```

New proposal:

Some of these only make sense for certain particles (i.e. binding energy inside isotope). Easier to enforce if they all get a unique element

```
<mass>…</mass>   or perhaps  <atomicM
<massExcess>…</massExcess>
<bindingEnergyPerNucleon>…</bindingEnergyPerNucleon>
```

Quantities may contain an <uncertainty>. Current version looks similar to GPDC, but would like to revise both (further discussion in afternoon)

Current status:

```
<mass recommended='quantity[@label="atomic"]'>
  <double label="atomic" value="1.0089" unit="amu">
    <documentation> ...</documentation>
    <uncertainty pdf="normal" type="variance-" value="9e-4"/>
    <uncertainty pdf="normal" type="variance+" value="1.2e-3"/>
  </double>
</mass>
```

New proposal:

```
<double label="atomic" value="1.0089" unit="amu">
  <asymmetricUncertainty>
    <minus type="variance-"><double value="9e-4"/></minus>
    <plus type="variance><double value="1.2e-3"/></plus></asymmetricUncertainty>
  </double>
```

Wrap this inside <uncertainty> element?

In similar spirit, create more specific tags for different types of <decay>?

- Currently:

<decay mode="…">...</decay>

- Child elements may be different depending on the mode

- Should this become <gammaDecay>, <betaMinusDecay>, <alphaDecay>, etc.?
  - Downside: there are *lots* of decay modes, so number of elements grows substantially
  - But… codes need to support all those modes whether they are stored by attribute or element.
  - From code point of view, if we plan to have different classes for each type of decay, then we recommend giving them unique tags

—Overriding particle database inside a reactionSuite

Particle properties (especially mass) not always consistent throughout ENDF-6 file. GND doesn't currently support, but probably should

- Allow a <particleDatabaseOverride> element, where particle properties can be modified as needed?
  - Supports using different masses in one evaluation, but makes it explicit and easy to detect
  - Where should it be allowed? I propose only allowing it in the <resonances> (or possibly <resolved> and <unresolved>), plus once per <reaction> element. Otherwise we could end up with a big mess!

—ENSDF2XML

Aaron Hurst (LBNL) has proposed new XML-based hierarchy to replace ENSDF (nuclear structure) format

- New format called ‘ensdf2xml’. Goal is slightly different from reaction-oriented particle database: in addition to evaluated level schemes, also supports
  - Experimental spectra following reaction / decay,
  - Observed gammas, even if not placed in a level scheme,
  - Etc.
- Already partly implemented, including utility for automatically translating ENSDF->XML
  - ENSDF comment records sometimes contain important info, translator does not attempt to parse those comments yet
  - Reverse translation back to ENSDF discussed but not yet implemented
- Proposal has many similarities to the particle database, also some important differences
  - Can we / should we try to resolve differences, to make databases more similar?

Quick overview of ensdf2xml (as of Nov. 2015):

```
<endsf2xml>
  <database name="ENSDF"/>
  <identification> … including what nucleus, what process (decay, etc.), etc.
        For example, dataset = "240Pu A decay" … </identification>
  <history>  … author, type of evaluation, "cutoff" date, etc. … </history>
  …
  <parent id="Ba133" A="133">
    <level>
      <energy value="0" unit="keV">
        <uncertainty value="0" pdf="N/A"/></energy>
      <spin string="1/2" value="0.5" unit="hbar"/>
      <parity value="+"/>
      <halflife value="10.551" unit="y">
        <uncertainty value="0.011" pdf="normal"/></halflife>
      also <lifetime>, <Q-value>, <atomicIonizationState>, <spectroscopicFactor>, …
    </level>
```

Decays in ensdf2xml (as of Nov. 2015):

```
<parent id="Pb210" A="210">
  <level id="Pb210_e4" index="4">
    <energy value="1275" unit="keV">…</energy>
    …
    <decay mode="betaMinus">
      <betaEnergy value="None" unit="keV">…</betaEnergy>
      <betaIntensity value="30">…</betaIntensity>
      <logft value="10.3">…</logft>
      <forbiddenness record="2U" classification="second-forbidden unique"/>
      <assignment record="firm"/>
    </decay>
  </level>
</parent>
```

Decays in ensdf2xml (as of Nov. 2015):

```
<parent id="Pb210" A="210">
  <level id="Pb210_e4" index="4">
    <energy value="1275" unit="keV">…</energy>
    …
    <decay mode="betaMinus">
      <betaEnergy value="None" unit="keV">…</betaEnergy>
      <betaIntensity value="30">…</betaIntensity>
      <logft value="10.3">…</logft>
      <forbiddenness record="2U" classification="second-forbidden unique"/>
      <assignment record="firm"/>
    </decay>
  </level>
</parent>
```

Should SG38 specification also allow labeling assignments as 'firm', 'tentative', etc.?

Decays in ensdf2xml (as of Nov. 2015):

```
<parent id="Pb210" A="210">
  <level id="Pb210_e4" index="4">
    <energy value="1275" unit="keV">…</energy>
    …
    <decay mode="betaMinus">
      <betaEnergy value="None" unit="keV
      <betaIntensity value="30">…</betaIn
      <logft value="10.3">…</logft>
      <forbiddenness record="2U" classific
      <assignment record="firm"/>
    </decay>
  </level>
</parent>
```

Other decay modes are similar except for names:

'ECandBetaPlus',
'alpha' (has 'hindranceFactor'),
'delayedParticle' (has 'width' and 'angularMomentumTransfer'),
'gamma' (has 'multipolarity', 'coincidence', 'mixingRatio', 'totalICC', etc.)

ENSDF supports forcing asymmetric uncertainties back to symmetric:

```
<decay mode="gamma">
  <gammaEnergy value="53.1622" unit="keV">
    <uncertainty value="0.0006" pdf="normal"/>
  </gammaEnergy>
  <branchingRatio value="3.45">
    <uncertainty value="0.05" pdf="normal"/>
  </branchingRatio>
  <multipolarity value="M1+E2"/>
  <mixingRatio value="0.08" sign="None">
    <uncertainty upperBound="+0.02" lowerBound="-0.03" pdf="asymmetric">
      <symmetrizationMethods>
        <method1 value="0.075000">
          <uncertainty value="0.025000" pdf="normal"/>
        </method1>
        <method2 value="0.072021">
          <uncertainty value="0.025226" pdf="normal"/>
        </method2>
      </symmetrizationMethods>
    </uncertainty>
  </mixingRatio>
```

ENSDF has many 'normalization' options: decay probability multipliers

<normalization>
  <NR … (photon intensity multiplier) …/>
  <NT … (transition intensity multiplier) …/>
  <BR … (branching ratio multiplier) …/>
  <NB … (beta multiplier) …/>
  <NP … (delayed particle multiplier …/>
</normalization>
  OR
<productionNormalization>
  <NRBR … (product of NR and BR above) …/>
  <NTBR … etc.

not sure what all these mean…

- Particle database does all of this differently: lists each decay mode (i.e. gamma vs internal conversion) on its own, with associated probability

ensdf2xml currently defining its own standard for bibliographic info

```
<references>
  …
  <reference index="362">
    <mass A="26"/>
    <keynumber id="2015KO08"/>
    <ref id="JOUR PRVCA 91 03423"/></reference></references>
```

- Aaron and I discussed possibility of using BibTeXML as standard bibliography layout.
  - ENSDF bibliographic info is very terse, expanding to full bibliography may require lots of effort

Final thoughts on similarities between ENSDF2XML and reaction-oriented particle database

- ENSDF2XML still in planning phase, we have held several discussions at LBNL looking for common elements.

- Overall goals are different, and format design will reflect that
  - In ENSDF, information about one isotope may be spread across several evaluations (especially if it is populated by more than one decay); particle database represents all in one place

- However, we are trying to standardize the basic ‘building blocks’ for both formats
  - bibliography,
  - representation of data and uncertainties
  - Particle naming conventions
  - ‘qualifiers’ (if needed)