Particle database
Requirements and Specifications

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Motivation:

- Design a unified structure for storing data about the particles and materials that appear in evaluated nuclear data libraries
  - Database will be mostly made up of nuclei and excited states, but also must handle photons, electrons, muons, atoms, molecules, etc.
  - Properties to be stored include mass, spin, charge, half-life, decay data including branching ratios and probabilities, as well as unique ids for each particle/material

Outline:

- Scope
- Proposed Requirements
- ‘ID’s
- Qualifiers
- Uncertainties

- Example of current implementation

Scope of the new database:

- In the short term, handle all data stored in:
  - RIPL masses and levels sub-directories,
  - ENDF atomic relaxation sub-libraries
  - ENDF decay sub-library

- Longer term:
  - Extend to ENSDF-style data? Requires more discussion with ENSDF community
  - Particle Data Group?

Proposed Requirements

- Each ‘matter’, ‘particle’ and ‘alias’ instance in the database shall have a unique id used to identify and refer to it. Only these classes shall have ids (for example, no id is given to the mass or spin, only to the instance itself).

- Every particle shall contain at least the following properties: mass, charge, spin, parity and half-life (which may be ‘stable’). However, some of these properties may be inherited from higher in the hierarchy rather than being listed explicitly

- The database shall support storing uncertainties with all particle properties. Multiple types of uncertainty should be supported, including central values with uncertainty, asymmetric distributions, and lists of multiple possible assignments. If multiple assignments are listed, the database shall require that one assignment be explicitly listed as the ‘recommended’ value.

- The database shall use nesting and inheritance where possible to reduce redundancy by grouping similar particles together.

- The database shall support defining ‘families’ to classify similar particles. Each particle family may have additional required data elements

Proposed Requirements (continued)

- The database shall support storing decay properties for unstable particles. Decays are organized into decay channels, which consist of a probability and a list of products.

- The database shall support storing documentation sections inside (at least) each particle and each property within that particle.

- The database shall support a bibliography section. Each item in the bibliography shall include a unique citation label that can be used to refer to it from any documentation section.

- The database shall support a section that defines a list of aliases for particles. For example, the id "Am242_m1" could be an alias for "Am242_e2".

- When linking to a particle database, user codes shall be permitted to add extra information about a particle by using ‘qualifier’ keys. For example, a qualifier key may be defined to describe the electron configuration of an atom following a photo- atomic reaction.

- Changes/additions to requirements?
  - Completeness criteria?

The database assigns unique ‘id’s to each particle and material. External codes use ids to refer to specific instances

- Unique id is assigned to each:
  - particle (e.g., ‘Fe56_e0’ for ground state of Iron-56, ‘e-’ for the electron, ‘photon’, etc.)
  - alias (e.g., ‘a’ for alpha particle, ‘t’ for triton, ‘Fe56’ as alternative name for ‘Fe56_e0’, etc.)
  - matter (e.g., ‘Fe’ for elemental iron)

- May also need unique ‘bibId’ for bibliography entries

‘Matter’ instance may contain ‘particle’ instances:

```
<chemicalElement id=“Mn” name=“Manganese” Z=“25”>
    <isotope name=“Mn48” A=“48”>
        <mass>...</mass>
        <nuclearLevel id=“Mn48_e0” index=“0” alias=“Mn48”>
            ...</nuclearLevel>
        <nuclearLevel id=“Mn48_e1” index=“1”>
            ...</nuclearLevel>
        ...</isotope>
    <isotope name=“Mn49” A=“49”>
    ...
</chemicalElement>
```

‘Matter’ instance may contain ‘particle’ instances:

```
<chemicalElement id="Mn" name="Manganese" Z="25">
    <isotope name="Mn48" A="48">
        <mass>...</mass>
        <nuclearLevel id="Mn48_e0" index="0" alias="Mn48">
            ...</nuclearLevel>
        <nuclearLevel id="Mn48_e1" index="1">
            ...</nuclearLevel>
        ...</isotope>
    <isotope name="Mn49" A="49">
    ...
</chemicalElement>
```

What if an excited state decays via internal conversion, kicks out an electron?

Can't assign unique levels to every possible combination of nuclear excited states and atomic configurations.
Proposed solution: store atomic (and other) data using 'qualifiers'

- Qualifiers are key/value pairs. The key can be appended to an id to supply extra information
  - id{qualifier}, as in 'U235{+2}', 'Fe56{1s1/2}'

- Qualifier values can be defined at multiple levels
  - For example, '+2' defined library-wide to mean 'missing 2 outermost electrons'
  - '1s1/2' defined at the <chemicalElement> level to mean 'missing electron from given subshell', along with atomic relaxation information

Syntax for qualifiers still needs to be expanded

- Allow multiple qualifiers to modify one id?
  - Yes: may need to specify multiple electron vacancies
- Support molecular configurations (important for thermal scattering sublibrary) through qualifiers?
  - Unsure. Libraries only contain a few molecular materials, may be easier to store them as ‘matter’ with their own ids

<uncertainty> elements

- Simple uncertainties like “3.157 +/- 0.024” can be stored using xml attributes:

  <quantity value=“3.157” uncertainty=“0.024”/>

- However, uncertainties can become much more complex: asymmetric distributions, confidence intervals, etc.

- For consistency, propose <uncertainty> always be stored in its own element.
  - Simplest version:

    <quant value=“...”><uncertainty value=“...” type=“normal”/></quant>

    May become more complicated:

    <quant value=“...”>
    <uncertainty type=“confidinceIntervals”>
    <confidenceInterval level=“66%” lower=“...” upper=“...”/>
    <confidenceInterval level=“95%” lower=“...” upper=“...”/>
    </uncertainty></quant>

- Li-7 example (nuclear excited states and decays)
  - Data taken from RIPL and AME
- Atomic relaxation
  - Data from ENDF atomic relaxation sub-library
- Still needed: translation of ENDF decay sub-lib
- How to tie these ingredients together?

```xml
<?xml version="1.0" encoding="UTF-8"?>
<particleDatabase formatVersion="0.1" library="RIPL+AME" libraryVersion="1.0" date="2014_10_23">
  <documentation>Sample particle database, generated by translating the RIPL3 levels file + AME masses for Li7.
    This example contains some tags not yet included in the requirements/specifications document, in particular
    the 'separationEnergies' element inside the nuclearLevel Li7_e0, the 'internalConversionCoefficient'.</documentation>
  <bibliography>
    <reference bibid="AME2003" genre="article" title="The Ame2003 atomic mass evaluation (II)" journal="Nuclear Physics"
    <reference bibid="RIPL3" genre="library"/></bibliography>
  <defaults>
    <!-- set default units if desired, and default uncertainty set to 'normal distribution' -->
    <default quantity="spin" unit="hbar"/>
    <default quantity="uncertainty" type="normal"/></defaults>
  <qualifiers>
    <qualifier key="+1" missingOutermostElectrons="1"/>
    <qualifier key="+2" missingOutermostElectrons="2"/>
    <qualifier key="u" unknownNuclearLevel="true"/></qualifiers>
  <aliases>
    <!-- create aliases for alpha and triton -->
    <alias id="a" pid="He4{+2}"/>
    <alias id="t" pid="H3{+1}"/></aliases>
  ...
  <chemicalElement id="Li" Z="3" name="Lithium">
    <isotope name="Li7" A="7">
      <mass value="7.016004548" unit="amu">
        <uncertainty value="8.4e-8"/>
        <alternateRepresentations>
          <mass value="14908.141" unit="keV" type="massExcess">
            <uncertainty value="0.079"/></mass>
          <mass value="5606.291" unit="keV" type="bindingEnergyPerNucleon">
            <uncertainty value="0.011"/></mass></alternateRepresentations></mass>
      <!-- levelScheme gives meta-data about how well-known the excited states are:
          some levels may be included even though complete experimental evidence not available -->
      <levelScheme maxCompleteUpTo="Li7_e0" uniqueSpinAndParityUpTo="Li7_e7"/>
      <nuclearLevel id="Li7_e0" index="0" alias="Li7">
        <energy value="0" unit="MeV"/>
        <spin value="1.5"/>
        <parity value="-"/>
        <halfLife value="stable" unit=""/>
        <separationEnergies>
           <neutron value="7.2499" unit="MeV"/>
           <proton value="9.975401" unit="MeV"/></separationEnergies></nuclearLevel>
      <nuclearLevel id="Li7_e1" index="1">
        <energy value="0.477612" unit="MeV"/>
        <spin value="0.5"/>
        <parity value="-"/>
        <halfLife value="7.3e-14" unit="s"/>
```

```
    <nuclearLevel id="Li7_e1" index="1">
      <energy value="0.477612" unit="MeV"/>
      <spin value="0.5"/>
      <parity value="-"/>
      <halfLife value="7.3e-14" unit="s"/>
      <decays>
        <decay index="0" mode="internalTransition">
          <probability value="1" unit=""/>
          <internalConversionCoefficient value="7.892e-7" unit=""/>
          <product index="0" pid="Li7_e0"/>
          <product index="1" pid="photon">
            <energy value="0.478" unit="MeV"/></product></decay></decays></nuclearLevel>
    <nuclearLevel id="Li7_e2" index="2">
      <energy value="4.63" unit="MeV"/>
      <spin value="3.5"/>
      <parity value="-"/>
      <halfLife value="4.91e-21" unit="s"/>
      <decays>
        <decay index="0" mode="alpha">
          <probability value="0.05" unit=""><uncertainty type="unknown"/></probability>
          <product index="0" pid="a"/>
          <product index="1" pid="t"/>
          <product index="2" pid="e-">
            <multiplicity value="3"/></product></decay>
        <decay index="1" mode="internalTransition" probability="0.95">
          <internalConversionCoefficient value="1.927e-8" unit=""/>
          <product index="0" pid="Li7"/>
          <product index="1" pid="photon">
            <energy value="4.628" unit="MeV"/></product></decay></decays></nuclearLevel>
    <nuclearLevel id="Li7_e3" index="3">
      <energy value="6.68" unit="MeV"/>
      <spin value="2.5"/>
      <parity value="-"/>
      <halfLife value="5.19e-22" unit="s"/>
      <decays>
        <decay index="0" mode="alpha">
          <probability value="1.0" unit=""><uncertainty type="unknown"/></probability>
          <product index="0" pid="a"/>
          <product index="1" pid="t"/>
          <product index="2" pid="e-">
            <multiplicity value="3"/></product></decay></decays></nuclearLevel>
    <nuclearLevel id="Li7_e4" index="4">
      <energy value="7.4595" unit="MeV"/>
      <spin value="2.5"/>
      <parity value="-"/>
      <halfLife value="5.13e-21" unit="s"/>
```

```
<element id="C">
  <configurations>
    <atomicConfiguration subshell="1s1/2" bindingEnergy="291.01 eV" electronNumber="2.0">
      <decay probability="0.000561488">
        <daughter particle="photon"/>
        <daughter particle="C{2p1/2}"/></decay>
      <decay probability="0.0011206">
        <daughter particle="photon"/>
        <daughter particle="C{2p3/2}"/></decay>
      <decay probability="0.413609">
        <daughter particle="e-"/>
        <daughter particle="C{2s1/2,2s1/2}"/></decay>
      <decay probability="0.13619">
        <daughter particle="e-"/>
        <daughter particle="C{2s1/2,2p1/2}"/></decay>
      <decay probability="0.271099">
        <daughter particle="e-"/>
        <daughter particle="C{2s1/2,2p3/2}"/></decay>
      <decay probability="0.00420748">
        <daughter particle="e-"/>
        <daughter particle="C{2p1/2,2p1/2}"/></decay>
      <decay probability="0.110012">
        <daughter particle="e-"/>
        <daughter particle="C{2p1/2,2p3/2}"/></decay>
      <decay probability="0.0632008">
        <daughter particle="e-"/>
        <daughter particle="C{2p3/2,2p3/2}"/></decay></atomicConfiguration>
    <atomicConfiguration subshell="2p1/2" bindingEnergy="8.99 eV" electronNumber="0.67"/>
    <atomicConfiguration subshell="2p3/2" bindingEnergy="8.98 eV" electronNumber="1.33"/>
    <atomicConfiguration subshell="2s1/2" bindingEnergy="17.56 eV" electronNumber="2.0"/></configurations></element>
```