## **Lawrence Livermore National Laboratory**

# **Unified particle properties database**



#### **Caleb Mattoon**

LLNL-PRES-636856

This work performed under the auspices of the U.S. Department of Energy by Lawrence Livermore National Laboratory under Contract DE-AC52-07NA27344

Nuclear reaction evaluations need particle property data as inputs. Rather than keeping multiple copies of this data, should have one central database.

 Current status in ENDF and GND: each file stores its own set of particle info.

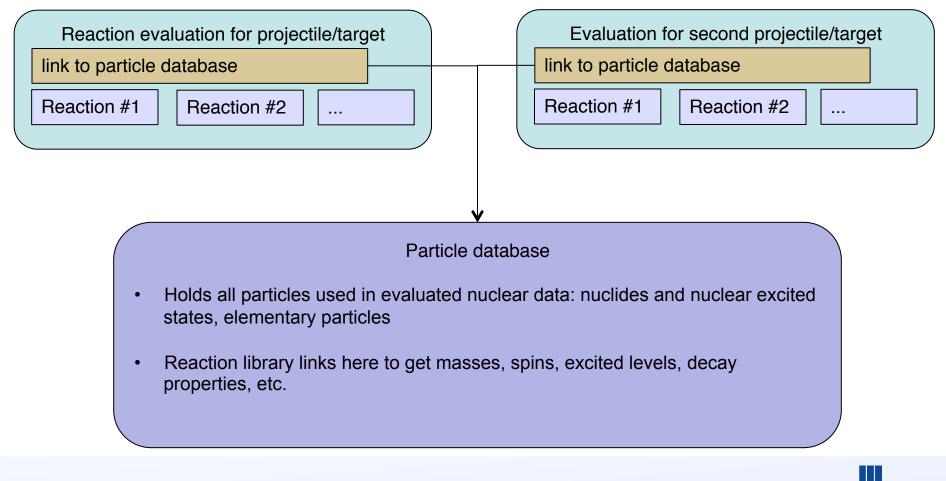
Reaction evaluation for projectile/targe						
list of particle info for this evaluation						
Reaction #1	Reaction #2					

(	Evaluation 1	tile/target	
	list of particle in	ation	
	Reaction #1	Reaction #2	



Nuclear reaction evaluations need particle property data as inputs. Rather than keeping multiple copies of this data, should have one central database.

 Current status in ENDF and GND: each file stores its own set of particle info. In future, replace that with a link:



### Why not use RIPL and the AME for the particle database?

- In the short term, that is probably the best solution. However,
  - We should translate this into a more human-readable hierarchy. Quoting from the SG38 requirements document:
    - "Use a hierarchy that reflects our understanding of nuclear (reactions and) decays, and that clearly and uniquely specifies all data."
  - Also, hierarchy should be extensible, to allow including other types of data (from ENSDF, for example)



## **Proposed schedule:**

20 Ma	13 ay Nov	-	14 ay No	20 Dv Ma	-
	Review POP, ENSDF, RIPL, masses,	First draft documenting structure	Second draft documenting structure	Release structure documentation	
			beta release of particle database	2 <sup>nd</sup> beta release of particle database	Release of particle database

- For the first milestone, we should review existing nuclear structure databases and decide:
  - what is the scope of the new database?
  - what elements from existing databases should be included?

#### What do we need in order to keep to this schedule?

- Need people (4-6) willing to spend time reviewing existing databases and come up with a plan for:
  - what data should be included
  - how that data should be organized
- Longer term, need to develop new tools to translate from existing databases into the new structure. Will need people to test these tools.

At LLNL we have already made some progress on designing a new hierarchy for particle properties, as well as an automatic translation tool.

- Reads RIPL and AME, translates into a new structure
- Every particle in the database has at least the following info:
  - A unique name to identify the particle
  - Mass (or energy if the particle is an excited state)
  - Halflife (or a flag for particles that are stable or very short-lived)
  - Spin / parity
  - Decay information if the particle is not stable
- For some particles, additional information may be available



- In addition to nuclei, a particle database should provide information about elementary particles (photons, electrons), mesons, and possibly some atomic information (such as electron binding energies)
- Should allow more complete decay information. For example, RIPL doesn't handle α- or β-decays to excited states, so β-delayed gamma info cannot be extracted

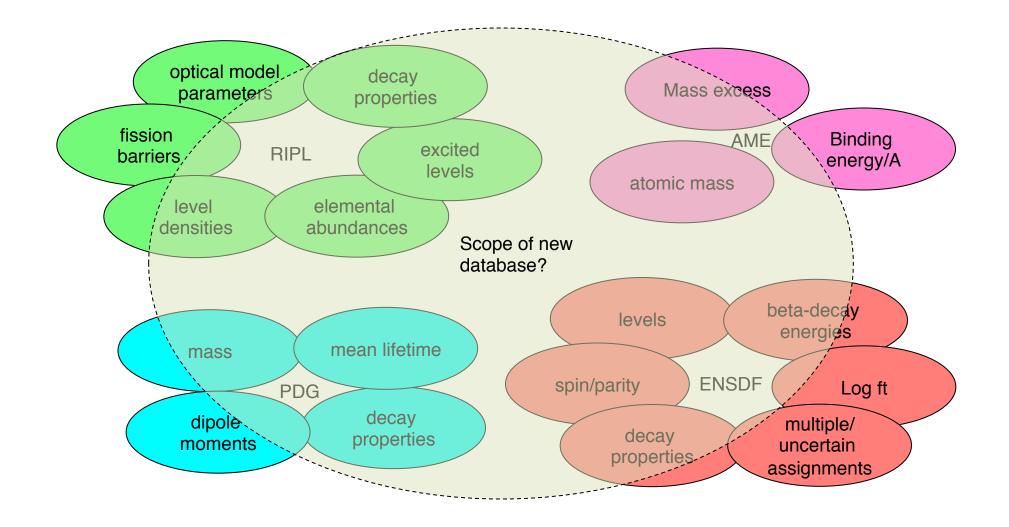


# Potential challenge if we start adding data from ENSDF: different philosophies behind RIPL and ENSDF

- If no measurements are available for a value, no assignment is made in ENSDF.
- RIPL builds upon ENSDF but makes additional assignments when possible so that computer codes always have a value to work with.
- Suggested resolution:
  - define a minimum set of properties that each particle (including excited states) must have, even if no experimental evidence is available.
  - Use a special flag to indicate when an assignment was made without direct evidence (RIPL already does this for spins)
  - Allow for other information beyond this minimum set of properties only when evidence is available



# Current databases store a wide range of data. Does the new database need to support all of these data, or just a subset?



### Some goals:

- The new structure for particle properties should
  - Store data in a structured hierarchy that mirrors nuclear structure physics
  - Build upon strengths of existing nuclear structure databases
  - Provide a way to link data and use aliases. For example, allow users to access metastable states either by metastable index or excitation level index
- Do we have any volunteers or recommendations to help with this task?
- Any other suggestions?



Extra slides



#### Sample of LLNL hierarchy in xml

```
<element name="O" Z="8">
 <natural>
   <abundance isotope="016" fraction="99.762" uncertainty="0.016"/>
   <abundance isotope="017" fraction="0.038" uncertainty="0.001"/>
   <abundance isotope="018" fraction="0.2" uncertainty="0.014"/></natural>
  <isotopes>
   <isotope name="O16" A="16">
    <mass value="15.99491461956" uncertainty="1.6e-10" unit="amu"/>
    <levels>
     <level name="016 e0" index="0">
       <energy value="0" unit="MeV"/>
       <spin value="0" parity="+"/>
       <halflife value="stable"/></nucleus></level>
     <level name="016 e1" index="1">
       <energy value="6.0494" unit="MeV"/>
       <spin value="0" parity="+"/>
       <halflife value="6.7e-11" unit="s"/>
       <decays>
         <decayMode type="gamma" branching="1.0">
          <product name="016 e0"/>
          cproduct name="photon"/></decayMode></decays></nucleus></level>
    </levels></isotope>
 </isotopes></element>
Lawrence Livermore National Laboratory
```



# More detail on ENSDF: originally designed to help automate publication of Nuclear Data Sheets.

- Data that can be stored in ENSDF include:
  - levels, gammas, bands, deformations, decay data, multipolarity, ...
- Problems with ENSDF:
  - Incomplete: values like spin, energy, etc. are left unassigned when no experimental data is available.
  - No version numbers
  - Not designed to be extensible. New types of data had to be added in comment fields, difficult to parse



# More about <u>RIPL</u>: designed to serve as input to modeling codes. Much more computer-readable than ENSDF, but doesn't handle as many types of data.

- RIPL defines a standard way to store level schemes, gamma decay information, level densities, optical model and deformation parameters, elemental abundances, fission barriers, ...
- RIPL starts with ENSDF values, and assigns values when ENSDF leaves blanks
- Includes a version number so users can link to a specific version
- Some problems:
  - Column-oriented format can be extended, but becomes more difficult to read as more data is packed in
  - Except for gamma decay, no way to specify when decay products are left in an excited state (i.e., beta/alpha decay)
  - Uncertainty / multiple assignments only supported for level energy and spins. More uncertainty options needed.

