General Purpose Data Containers

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May 9–13, 2016

LA-UR-16-23173

GND @ LANL

- We have begun to write code to read/parse GND at LANL
- Suggestions based on our experience

- GND is in a pretty good state
- Suggestions are more like refinements rather than big changes.

Hierarchy of Data Containers

Computer Science (level 0)

Storage of fundamental data types on a computer; e.g., numerical, text

Applied Mathematics (level 1)

Representations of mathematical concepts on a computer; e.g., series coefficients, grids, moments, indices

Physics (level 2+)

Representation of physical concepts, units, etc.

Hierarchy Rules to Live By

- Read/parse container context-free
- Read/parse container independently, regardless of location in file

- Add container only when context changes; i.e.,
  - CS
    - Integer vs floating point
  - math
    - Interpolation
    - Representation (e.g., Legendre, tabulated)
    - Higher dimension
    - Discontinuity
  - physics
    - Units
    - Processing

Why so many <regionxXd>

Simplified:

- parsing
- validation
- extension

Why so many <regionxXd>

When should a <regionsXd> be used?

- Primary container underneath physics level
- Lower-dimensional container(s) as children of higher-dimensional math container

Simplified:

- parsing
- validation
- extension

```
<XYs2d>
  <regions1d>
    <XYs1d>...</XYs1d>
    <XYs1d>...</XYs1d>
  </regions1d>
  <regions1d>
    <Legendre>...</Legendre>
  </regions1d>
</XYs2d>
```

Cross Section

1 Region

Single Region

```
<crossSection>
  <axes>
    <axis index="1" label="energy_in" unit="eV"/>
    <axis index="0" label="crossSection" unit="b"/></axes>
  <regions1d label="eval">
    <XYs1d> <values> 1E-5 15 ... 1E-3 13 </values> </XYs1d>
    <!-- Note the double value -->
    <XYs1d> <values> 1E-3 10 ... 2E7 13 </values> </XYs1d>
  </regions1d>
</crossSection>
```

Cross Section

Multiple Regions

Multiple Regions

```
<crossSection label="eval">
  <axes>
    <axis index="1" label="energy_in" unit="eV"/>
    <axis index="0" label="crossSection" unit="b"/>
  </axes>
  <resonancesWithBackground>
    <resonanceRegion xlink:href="/reactionSuite/resonances"/>...
  </resonancesWithBackground>
  <regions1d>
    <XYs1d><values> 1E-5 10 ... 2E-5 13 </values></XYs1d>
    <XYs1d><values> 2E-5 10 ... 2E7 13 </values></XYs1d>
  </regions1d>
</crossSection>
<crossSection label="recon">...</crossSection>
```

Angular Probability Distribution

Legendre

```
<distribution>
  <angularTwoBody label="eval" productFrame="centerOfMass">
    <axes>
      <axis index="2" label="energy_in" unit="eV"/>
      <axis index="1" label="mu" unit=""/>
      <axis index="0" label="P(mu|energy_in)" unit="1/eV"/>
    </axes>
    <regions2d interpolation="lin-lin">
      <XYs2d>
        <regions1d value="1e-5"><Legendre> ... </Legendre>...</regions1d>
          ...
        <regions1d value="2e7"><Legendre> ... </Legendre>...</regions1d>
      </XYs2d>
    </regions2d>
  </angularTwoBody>
</distribution>
```

Angular Probability Distribution

Single Tabulated Region

Tabulated

```
<distribution>
  <angularTwoBody label="eval" productFrame="centerOfMass">
    <axes>
      <axis index="2" label="energy_in" unit="eV"/>
      <axis index="1" label="mu" unit=""/>
      <axis index="0" label="P(mu|energy_in)" unit="1/eV"/></axes>
    <regions2d interpolation="lin-lin">
      <XYs2d>
        <regions1d value="1e-5"><XYs1d> ... </XYs1d>...</regions1d>
          ...
        <regions1d value="2e7"><XYs1d> ... </XYs1d>...</regions1d>
      </XYs2d>
    </regions2d>
  </angularTwoBody>
</distribution>
```

Angular Probability Distribution

Change of Representation/Units

```
<distribution>
  <angularTwoBody label="eval" productFrame="centerOfMass">
    <axes>
      <axis index="2" label="energy_in" unit="eV"/>
      <axis index="1" label="mu" unit=""/>
      <axis index="0" label="P(mu|energy_in)" unit="1/eV"/></axes>
    <regions2d>
      <XYs2d interpolation="lin-lin">
        <regions1d value="1e-5"><Legendre> ... </Legendre></regions1d>
            ...
        <regions1d value="5e6"><Legendre> ... </Legendre></regions1d>
      <!-- Change in representation -->
        <regions1d value="6e6"><XYs1d> ... </XYs1d>...</regions1d>
          ...
        <regions1d value="2e7"><XYs1d> ... </XYs1d>...</regions1d>
      </XYs2d>
    </regions2d>
  </angularTwoBody>
</distribution>
```

Double-Differential Disribution

Mixed Representation

Double Differential Distribution

```
<!-- Modified from Fe-56, MT=28 -->
<distribution>
  <energyAngular label="eval" productFrame="lab">
    <axes>
      <axis index="3" label="energy_in" unit="eV"/>
      <axis index="2" label="energy_out" unit="eV"/>
      <axis index="1" label="mu" unit=""/>
      <axis index="0" label="P(mu|(energy_out|energy_in))" unit="1/eV"/>
    </axes>
    <XYs3d interpolationQualifier="correspondingPoints">
      <regions2d>
        <XYs2d value="10364000.0" interpolation="flat">
          <regions1d>
            <XYs1d value="0.0"><Legendre>...</Legendre>...
            <XYs1d value="1e-05"><Legendre>...</Legendre>
        </regions1d></XYs2d>
        <XYs2d value="11500000.0" interpolation="flat">
          <regions1d>
            <XYs1d value="0.0"><Legendre>...</Legendre> ...
            <XYs1d value="375000.0"><Legendre>...</Legendre>
        </regions1d></XYs2d>
        <!-- Change in interpolation -->
        <XYs2d value="11600000.0" interpolation="flat">
          <regions1d>
            <XYs1d value="0.0"><Legendre>...</Legendre> ...
            <XYs1d value="525000.0"><Legendre>...</Legendre>
        </regions1d></XYs2d>
      </regions2d>
  </XYs3d></energyAngular></distribution>
```

Conclusion

- GND version 1.7 is pretty good
- Pay attention to the container hierarchy:
  - computer science
  - math
  - physics
- Add containers when context changes
- Utilize `<regionsXd>` containers for simplification of parsing, validating, and extending.