GND: Storing multiple representations of a quantity using forms, components and styles

Presented WPEC Sub-group 38

May 2016

Bret Beck

Lawrence Livermore National Laboratory

LLNL-PRES-??????

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

Outline

- Why components, forms and styles are needed
- What is a component?
  - An object that stores a quantity
- What is a form?
  - One representation of a quantity. There can be more than one in a component.
- What is a style?
  - A place to store common information about related forms
- Examples
- Some style types

Bit of history

Evaluation MC Pn

All have the same structure down to the data level

Why components, forms and styles are needed

- In addition to storing evaluation data, we want to be able to store multiple ‘processed’ data simultaneously
- What are ‘processed data’
  - Different representations of a quantity more useful for people to view or for use in transport codes
  - Examples:
    - Pointwise cross section reconstructed from resonances data
    - Heated cross section
    - Multi-grouped data (cross section, distribution, etc.)
- Example for cross section
  - Resonance data, reconstructed, heated to 1 eV, heated to 10 eV, 1 eV multi-grouped

What is a component?

- A quantity is dependent on the projectiles energy
  - So far this fits all components in GND
- It stores a list of forms for that quantity
- Examples are
  - The cross section for a reaction: $\sigma(E)$
  - The Q value for a reaction channel: Q(E)
    - Note, “value” makes it sound like a single number. It would be if we could do the physics correctly then, we would not need to store it as a component
  - The multiplicity for an outgoing particle: m(E)
    - See Q value note.
  - Average energy and momentum to an outgoing particle: E’(E) and p’(E)
  - Available energy and momentum to an outgoing particle: $E_{available}(E)$ and $p_{available}(E)$
  - Outgoing particle distribution: $P(E',\mu|E)$
  - Currently, that what is in GND but there may be others

What is a form?

- Different representations of the “same” quantity (component)
  - What about multi-group data? E.g., distribution weighted by cross section. Should data be unitless or ‘b’?
- Example for a cross section
  - Form 1) Evaluation form may be resonances with background
  - Form 2) This (Form 1) can be converted to a lin-lin pointwise representation
  - Form 3) Form 2 can be heated to 1 eV
  - Form 4) Form 3 multigrouped
  - Form 5) Form 2 can be heated to 10 eV
  - Form 6) Form 5 multigrouped
- Need a way to distinguish the forms

Multi-grouped distribution

Data from different components

$$\frac{\int dE \int dE' \int d\mu\, \sigma_s(E)\, P(\mu, E' \mid E)\, f(E)}{\int dE\, f(E)}$$

Not part of any components

$$\frac{\int dE \int dE' \int d\mu\, \sigma_s(E)\, P(\mu, E' \mid E)\, f(E)}{\int dE\, \sigma_s(E)\, f(E)}$$

Multi-grouped distribution data are stored in the distribution component.

What is a style?

- Represents a set of forms that were all processed the same way
  - Defines a unique label that all of its forms have
  - Example of common processing:
    - Multi-grouping data with a given temperature and group boundaries
- A place to store information common to various processed data to reduce redundancy
  - Examples of data stored:
    - Cross section heating
      - Temperature
    - Multi-grouping
      - Group boundaries and flux used

Time for some examples

Example of cross section with 5 forms

```
- <reactionSuite projectile="n" target="U233" version="GND 1.7" projectileFrame="lab">
  - <styles>
      <evaluated label="eval" library="ENDF/B" version="7.1.1" date="2006-09-01" temperature="0. K"/>
      <crossSectionReconstructed label="recon" date="2016-03-30"/>
      <heated label="h1" temperature="1. eV" date="2016-03-30"/>
      <heated label="h2" temperature="10. eV" date="2016-03-30"/>
    + <SnMultiGroup label="Sn" lMax="3" date="20150101"></SnMultiGroup>
    </styles>
  + <documentations></documentations>
  + <particles></particles>
  + <resonances reconstructCrossSection="true"></resonances>
  - <reactions>
    - <reaction label="0" outputChannel="n + U233" date="2006-09-01" ENDF_MT="2">
      - <crossSection>
          + <resonancesWithBackground label="eval"></resonancesWithBackground>
          + <XYs1d label="recon"></XYs1d>
          + <XYs1d label="h1" accuracy="0.002"></XYs1d>
          + <XYs1d label="h2" accuracy="0.002"></XYs1d>
          + <gridded1d label="Sn"></gridded1d>
        </crossSection>
      + <outputChannel genre="twoBody"></outputChannel>
      </reaction>
    </reactions>
  + <sums></sums>
  + <fissionComponents></fissionComponents>
</reactionSuite>
```

Description of some styles: Proposed and their members

Some comments first

- The following examples are currently implemented in FUDGE but not cast in stone.

- These examples are missing information about the processing code(s).
  - That is, they should contain something like a <codes> element that would have code name, version and may the input parameters

Evaluated style

- Members
  - label
  - date
  - library
  - Version
  - temperature

Common to all styles

```
<evaluated label="eval”
           date="2006-09-01”
           library="ENDF/B”
           version="7.1.1”
           temperature="0. K"></evaluated>
```

crossSectionReconstructed style

- label
- date

```
<crossSectionReconstructed
        label=”recon”
        date="2016-05-06”></crossSectionReconstructed>
```

angularDistributionReconstructedstyle

- label
- date

Heated style

- label
- date
- temperature

```
<heated label="h1”
        temperature="1. eV”
        date=” 2016-05-06”</heated>
```

averageProductData style

- label
- date

SnMultiGroup style (1/2)

- Label
- date
- Maximum Legendre order
- Sub-elements
  - flux
  - Transportables (list of particles processed)
    - List of transportable
      - Groups (defines group boundaries for each particle)

SnMultiGroup style (1/2)

```
<SnMultiGroup          label=”Sn”
                       lMax=”3
                       date=” 2016-05-06”>
   <flux label="LLNL_fid_1">
      <fluxOrder order="0">
         <XYs1d>
            <axes>
               <axis index="1" label="energy_in" unit="eV"/>
               <axis index="0" label="flux" unit="1/s"/></axes>
            <values>0 85 2.1e7 85</values></XYs1d></fluxOrder></flux>

   <transportables>
      <transportable label="He4" conserve="number">
         <group label="He4" gid="LLNL_gid_71">
            <grid index="0" label="energy_in" unit="eV" style="boundaries">
               <values length="64">1e-4 2e4
                  . . . </values></grid></group></transportable>
      <transportable label="He3" conserve="number"> . . . </transportable>
      <transportable label="H3" conserve="number"> . . . </transportable>
      <transportable label="H2" conserve="number"> . . . </transportable>
      <transportable label="H1" conserve="number"> . . . </transportable>
      <transportable label="n" conserve="number"> . . . </transportable>
      <transportable label="gamma" conserve="number"> . . . </transportable>
                                 <transportables></SnMultiGroup>
```