Brainstorming GND Markup for Fission Product Yields

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The Generalized Nuclear Data (GND) format is a possible replacement for the ENDF format

- Under active development under auspices of WPEC/ SG-38
- Lead by D. McNabb, outgrowth of earlier LLNL (US) project
- Initial focus was neutron and charged particle transport data
- Now looking to other ENDF format/data, in particular, FPY formats

Fission Product Yield tables give the number of nuclides of a given type, post-fission

- **Independent Fission Product Yields (IFPY)**
  These are the fragments immediately after fission and de-excitation from prompt neutron and gamma emission
- **Cumulative Fission Product Yields (CFPY)**
  These are the fragments after they are allowed to undergo all (beta and other) decays
- If you think about it, if you know all possible decays of all fission products, you can construct a matrix that relates the IFPY and CFPY.
  - Both A. Sonzogni and R. Mills have codes that can compute this matrix from the decay sublibrary
  - Implies only one of IFPY and CFPY needed

There are two MT's in ENDF that use the same FPY format. MT=454 is IFPY and MY=459 is CFPY.

8.3.1 Formats

The structure of a section always starts with a HEAD record and ends with a SEND record. Sets of fission product yield data are given for one or more incident energies. The sets are ordered by increasing incident energy. For a particular energy the data are presented by giving four parameters (ZAFP, FPS, YI, and DYI in MT=454 and ZAFP, FPS, YC, and DYC in MT 459) for each fission product state. The data are first ordered by increasing values of ZAFP. If more than one yield is given for the same (Z,A) the data are ordered by increasing value of the state designator (FPS). The structure for a section is:

```
[MAT, 8, MT/ ZA, AWR, LE+1, 0,  0,   0]HEAD
[MAT, 8, MT/ E1, 0.0,   LE, 0, NN, NFP/ Cn(E1) ]LIST
[MAT, 8, MT/ E2, 0.0,    I, 0, NN, NFP/ Cn(E2) ]LIST
[MAT, 8, MT/ E3, 0.0,    I, 0, NN, NFP/ Cn(E3) ]LIST
  ------------------------
[MAT, 8, 0 /0.0, 0.0,    0, 0,  0,   0]SEND
```

where MT=454 for independent yield data, and MT=459 for cumulative yield data. There are (LE+1) LIST records.

fudge/legacy/converting/endfFileToGND.py has readMF8 function

This is what the ENDF parameters mean (part 1)

NFP Number of fission product nuclide states to be specified at each incident energy point (this is actually the number of sets of fission product identifiers fission product yields). (NFP$\leq$ 2500).

ZAFP (Z,A) identifier for a particular fission product. (ZAFP = $(1000Z + A)$).

FPS State designator (floating-point number) for the fission product nuclide (FPS = 0.0 means the ground state, FPS=1.0 means the first excited state, *etc.*)

YI (MT=454), independent yield for a particular fission product prior to particle decay.

DYI (MT=454) 1σ uncertainty in YI.

YC (MT=459) cumulative yield.

DYC (MT=459) 1σ uncertainty in YC.

This is what the ENDF parameters mean (part 2)

$C_n(E_i)$ Array of yield data for the i^{th} energy point. This array contains NFP sets of four parameters in the order ZAFP, FPS, YI, and DYI in MT=454 and ZAFP, FPS, YC, and DYC in MT=459.

NN Number of items in the $C_n(E_i)$ array, equal to 4*NFP.

E_i Incident particle energy of the i^{th} point (eV).

LE Test to determine whether energy-dependent fission product yields given:

- LE=0 implies no energy-dependence (only one set of fission product yield data given);
- LE>0 indicates that (LE+1) sets of fission product yield data are given at (LE+1) incident particle energies.

I_i Interpolation scheme (see paragraph on Two-dimensional Interpolation Schemes in Section 0.5.2) to be used between the E_{i-1} and E_i energy points.

Where can we put this and how?

- **Both IFPY and CFPY are reaction data.**
  They should be part of a <reactionSuite> in the fission <reaction>.

- **Do we need to store the matrix?**
  Currently no easy way to tell if IFPY and CFPY are internally consistent.

- **How do we store dY?**
  IFPY and CFPY both have Y and dY. GND currently doesn't have a provision for uncertainties along side the data.

- **What about full covariances?**
  Neither GND nor ENDF have provisions for them. In GND it is not hard to make a spot for them. Is there test data to use?

GND version should be part of the total fission <reaction>, even if rest of reaction unpopulated with data

```
1    <?xml version="1.0" encoding="UTF-8"?>
2  ▼ <reactionSuite projectile="n" target="Pu239" format="gnd version 1.2" temperature="0 K" xmlns:xlink="http://ww
3  ▶   <styles> ••• </styles>
5  ▶   <documentations> ••• </documentations>
40 ▶   <particles> ••• </particles>
43     <reaction label="45" outputChannel="n[multiplicity:'energyDependent', emissionMode:'prompt'] + n[emissionMod
...▼ [total fission]" date="2006-09-01" ENDF_MT="18" fissionGenre="total">
44 ▶     <crossSection nativeData="resonancesWithBackground"> ••• </crossSection>
65 ▼     <outputChannel genre="NBody" Q="1.98902e8 eV">
66 ▶       <fissionEnergyReleased nativeData="polynomial"> ••• </fissionEnergyReleased>
77 ▼       <fissionProductYields nativeData="independentFissionProductYields" conversionMatrixGiven="true">
78 ▶         <independentFissionProductYields numNuclides="780"> ••• </independentFissionProductYields>
95 ▶         <cumulativeFissionProductYields numNuclides="920"> ••• </cumulativeFissionProductYields>
11 ▶         <fissionYieldConversionMatrix> ••• </fissionYieldConversionMatrix>
28 ⌙       </fissionProductYields>
29 ▶       <product name="n" label="n" multiplicity="energyDependent" emissionMode="prompt"> ••• </product>
94 ▶       <product name="n" label="n__a" multiplicity="energyDependent" decayRate="0.013271 1/s" emissionMode="del
35 ▶       <product name="n" label="n__b" multiplicity="energyDependent" decayRate="0.030881 1/s" emissionMode="del
76 ▶       <product name="n" label="n__c" multiplicity="energyDependent" decayRate="0.11337 1/s" emissionMode="dela
29 ▶       <product name="n" label="n__d" multiplicity="energyDependent" decayRate="0.2925 1/s" emissionMode="delay
82 ▶       <product name="n" label="n__e" multiplicity="energyDependent" decayRate="0.85749 1/s" emissionMode="dela
35 ▶       <product name="n" label="n__f" multiplicity="energyDependent" decayRate="2.7297 1/s" emissionMode="delay
88 ▶       <product name="gamma" label="gamma" multiplicity="energyDependent"> ••• </product></outputChannel></react
12 ⌙   </reactionSuite>
13
```

GND version should be part of the total fission <reaction>, even if rest of reaction unpopulated with data

```
<?xml version="1.0" encoding="UTF-8"?>
<reactionSuite projectile="n" target="Pu239" format="gnd version 1.2" temperature="0 K" xmlns:xlink="http://ww
  <styles> … </styles>
  <documentations> … </documentations>
  <particles> … </particles>
  <reaction label="45" outputChannel="n[multiplicity:'energyDependent', emissionMode:'prompt'] + n[emissionMod
[total fission]" date="2006-09-01" ENDF_MT="18" fissionGenre="total">
    <crossSection nativeData="resonancesWithBackground"> … </crossSection>
    <outputChannel genre="NBody" Q="1.98902e8 eV">
      <fissionEnergyReleased nativeData="polynomial"> … </fissionEnergyReleased>
      <fissionProductYields nativeData="independentFissionProductYields" conversionMatrixGiven="true">
        <independentFissionProductYields numNuclides="780"> … </independentFissionProductYields>
        <cumulativeFissionProductYields numNuclides="920"> … </cumulativeFissionProductYields>
        <fissionYieldConversionMatrix> … </fissionYieldConversionMatrix>
      </fissionProductYields>
      <product name="n" label="n" multiplicity="energyDependent" emissionMode="prompt"> … </product>
      <product name="n" label="n__a" multiplicity="energyDependent" decayRate="0.013271 1/s" emissionMode="del
      <product name="n" label="n__b" multiplicity="energyDependent" decayRate="0.030881 1/s" emissionMode="del
      <product name="n" label="n__c" multiplicity="energyDependent" decayRate="0.11337 1/s" emissionMode="dela
      <product name="n" label="n__d" multiplicity="energyDependent" decayRate="0.2925 1/s" emissionMode="delay
      <product name="n" label="n__e" multiplicity="energyDependent" decayRate="0.85749 1/s" emissionMode="dela
      <product name="n" label="n__f" multiplicity="energyDependent" decayRate="2.7297 1/s" emissionMode="delay
      <product name="gamma" label="gamma" multiplicity="energyDependent"> … </product></outputChannel></react
</reactionSuite>
```

Proposed

From ENDF

In ENDF, both Y and dY stored, can we do that in an XY? Can we put multiple <data>'s in a <linear> block?

```
<independentFissionProductYields numNuclides="780">
    <linear xData="XYs" length="6" accuracy="0.001" hasUncertainty="true">
        <axes>
            <axis index="0" label="energy_in" unit="eV" interpolation="linear,flat" frame="lab"/>
            <axis index="1" label="yield" unit="" frame="lab"/></axes>
        <data nuclide="Nd146_e0">
                    1e-05 3.45996e-13 2.21437e-13
                   0.0253 3.45996e-13 2.21437e-13
                 500000.0 4.01972e-13 2.57262e-13
                2000000.0 4.01945e-13 2.57245e-13
               14000000.0 5.452814e-09 3.489803e-09
               20000000.0 5.452814e-09 3.489803e-09
               </data>
        <data nuclide="..."> ••• </data>
    </linear>
</independentFissionProductYields>
```

The optional matrix that couples the IFPY and the CFPY can be stored here too

```
<fissionYieldConversionMatrix>
    <!-- Each row of this matrix corresponds to a nuclide in the independentFissionProductYields and
         each column of this matrix corresponds to a nuclide in the cumulativeFissionProductYields.
         The ordering of nuclides is arbitrary, but it is more convienient if they match the ordering
         in the independentFissionProductYields and cumulativeFissionProductYields elements.

         Do we really need the URL and the xlink here?-->
    <rowParameters>
        <parameter name="Nd146_e0" xlink:href="../../independentFissionProductYields/linear/data[]"/>
        ...</rowParameters>
    <columnParameters>
        ...</columnParameters>
<matrix rows="780" columns="920" form="asymmetric" precision="6">
        0.000000e+00  ....
        0.000000e+00  6.367300e-04 ....
        ....
</matrix></fissionYieldConversionMatrix>
```

Should this be energy dependent?

Is this the best way?

On the issue of covariances...

- **For the individual yields**
  - It makes sense to have covariance for either IFPY or CFPY, then derive other
  - Simple covariance format can be created using existing GND covariance markup
- **Cross nuclide covariances**
  - Simple covariance format can also be created using existing GND covariance markup
- **Covariance on conversion matrix?**
  - Requires better covariances on data in decay sublibrary
  - If care about nuclei after heat death of universe, then T1/2's drop out. In real life, there are long lived isotopes that don't finish beta decaying by the time of the CFPY. Uncertainty propagation tough here since parameter dependence nonlinear.