Uncertainties and covariances in SG38 and GND-1.7

Joint meeting of WPEC subgroups 38, 39 and 40
May 20, 2015

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ENDF-VII.1 has been translated into the latest version (GND-v1.7), available on NNDCforge:

- ENDF-VII.1 neutron and standards sub-libraries are available in the latest GND format from https://ndclx4.bnl.gov/gf/project/gnd/scmgit/?p=gnd;a=tree

- Another Fudge release with GND-1.7 support is coming soon. It includes recent changes suggested by SG38 collaborators
SG38: overhaul how we store and use nuclear data, including uncertainties and covariances

- Some main goals:
  - Handle all data from ENDF-6, and maintain backwards-compatibility (translation to/from ENDF-6).
  - Make data easy to understand and use.
  - Design general-purpose low-level containers that can be reused to store different types of data.
  - Be flexible! Covariance needs are growing (thermal scattering, double-differential distributions, etc.), we need to be able to respond quickly.
    - Need input from WPEC on this: what new types of covariance data should be the first focus?
ENDF-6 support for covariances is a good start, but needs to be extended.

- **What ENDF-6 does well:**
  - General-purpose matrix containers are reused to store many different types of data.
  - Support for individual covariances + cross terms between different reactions and/or materials.

- **Weaknesses:**
  - Interpolation: ENDF-6 only supports ‘flat’ interpolation for cross section, multiplicity and energy/angle spectra.
  - No support for asymmetric or log-normal distributions, confidence intervals, etc.
  - General model-parameter covariances are ‘supported’ (MF=30) but not used in practice.
  - Limited ENDF-6 precision leads to numerical problems.
GND-1.7 handles nearly all ENDF-6 covariance data.

- Supported: fission neutron multiplicity (MF=31), resonance parameters (32)*, cross sections (33), angular distributions (34), energy distributions (35), production cross section (40)

- *Still unsupported: MF=32, LRF=7. New CIELO evaluations mean these are high priority!

- GND organizes uncertainty data inside ‘uncertainties’ and ‘covarianceSuite’ elements
GND 1.7 overview

- Within the GND `<reactionSuite>`, data are divided into reactions:

```xml
<reaction label="..." outputChannel="..." date="..." ENDF_MT="...">
  <crossSection> ... </crossSection>
  <!-- options: pointwise, piecewise, ‘resonancesWithBackground’ -->
  <outputChannel>
    <Q> <!-- constant, except for gammas and fission --> </Q>
    <product name="..." label="...">
      <distributions>...</distributions>
      <multiplicity>...</multiplicity></product>
    <product>...</product>
    ...
  </outputChannel>
</reaction>
```

---

**color code:**

- `element` attribute
- `attribute` comment
GND 1.7 overview

- Within the GND <reactionSuite>, data are divided into reactions:

```xml
<reaction label="..." outputChannel="..." date="..." ENDF_MT="...">
  <crossSection> ... </crossSection>
  <!-- options: pointwise, piecewise, 'resonancesWithBackground' -->
  <outputChannel>
    <Q> <!-- constant, except for gammas and fission --> </Q>
    <product name="..." label="...">
      <distributions>...</distributions>
      <multiplicity>...</multiplicity></product>
    </product> ...
  </outputChannel>
</reaction>
```

- <uncertainties> element can appear at several points
GND 1.7 overview

- Example: prompt fission neutron multiplicity data with covariance:

```xml
<product name="n" label="n" emissionMode="prompt">
  <multiplicity>
    <XYs style="eval">
      <axes>...</axes>
      <values length="5452">1e-5 2.8743 ... 2e+7 5.697</values>
      <uncertainties>
        <uncertainty type="covariance">
          <link xlink:href="/covarianceSuite/section[@label='1']"/>
          <!-- instead of link, could contain the actual matrix -->
        </uncertainty>
      </uncertainties>
    </XYs>
  </multiplicity>
</product>
```
Example: prompt fission neutron multiplicity data with covariance:

```xml
<product name="n" label="n" emissionMode="prompt">
  <multiplicity>
    <XYs style="eval">
      <axes>...</axes>
      <values length="5452">1e-5 2.87 ... 2e+7 5.697</values>
      <uncertainties>
        <uncertainty type="covariance">
          <link xlink:href="/covarianceSuite/section[@label='1']"/>
          <!-- instead of link, could contain the actual matrix -->
          <!-- instead of link, could contain the actual matrix -->
        </uncertainty>
      </uncertainties>
    </XYs>
  </multiplicity>
</product>
```

More than one ‘uncertainty’ element may live here, for example to support asymmetric upper/lower uncertainties.
Covariance matrices are stored in a ‘gridded’ container (energy boundaries + axis description + array)

```xml
<covarianceSuite projectile="n" target="Pu239" version="GND 1.7" xmlns:xlink="http://www.w3.org/1999/xlink">
    <section label="1" id="n + Pu239 [total fission] [nubar]" nativeData="covarianceMatrix">
        <rowData xlink:href="/reactionSuite/reaction[@label='45']/.../multiplicity" ENDF_MFMT="31,456"/>
        <covarianceMatrix type="relative">
            <gridded dimension="2">
                <axes>
                    <axis index="2" label="row_energy_bounds" unit="eV" gridStyle="boundaries"/>
                    <values length="11"> 1e-5 1e+5 5e+5 1e+6 2e+6 6e+6 1e+7 1.4e+7 1.6e+7 1.8e+7 2e+7 </values>
                    <axis index="1" label="column_energy_bounds" unit="eV" gridStyle="link"/>
                    <axis index="0" label="matrix_elements" unit=""/>
                </axes>
                <array shape="10,10" symmetry="lower">
                    1.743597e-04
                    2.356280e-04  3.184498e-04
                    1.378220e-04  1.863129e-04  2.404747e-04  2.648832e-04  2.672193e-04  2.506376e-04  2.174015e-04 ...
                    4.800182e-05  6.488835e-05  8.375597e-05  9.226280e-05  9.309246e-05  8.733193e-05  7.578035e-05 ...
                </array></gridded></covarianceMatrix></section>
</covarianceSuite>
```
Covariance matrices are stored in a ‘gridded’ container (energy boundaries + axis description + array)

```
<covarianceSuite projectile="n" target="Pu239" version="GND 1.7" xmlns:xlink="http://www.w3.org/1999/xlink">
  <section label="1" id="n + Pu239 [total fission] [nubar]" nativeData="covarianceMatrix">
    <rowData xlink:href="/reactionSuite/reaction[@label='45']/.../multiplicity" ENDF_MFMT="35,18"/>
    <covarianceMatrix type="relative">
      <gridded dimension="2">
        <axes>
          <axis index="2" label="row_energy_bounds" unit="eV" gridStyle="boundaries">
            <values length="11">1e-5 1e+5 5e+5 1e+6 2e+6 6e+6 1e+7 1.4e+7 1.6e+7 1.8e+7 2e+7</values></axis>
          <axis index="1" label="column_energy_bounds" unit="eV" gridStyle="link"/>
          <axis index="0" label="matrix_elements" unit=""/></axes>
        <array shape="10,10" symmetry="lower">
          1.743597e-04 2.356280e-04 3.184498e-04
          3.347426e-04 4.524720e-04 5.839602e-04
          3.376183e-04 4.563926e-04 5.890303e-04
          3.165935e-04 4.279883e-04 5.523777e-04
          2.745613e-04 3.711586e-04 4.790528e-04
          2.141380e-04 2.894741e-04 3.736303e-04
          1.378220e-04 1.863129e-04 2.404747e-04
          4.800182e-05 6.488835e-05 8.375597e-05
        </array></gridded></covarianceMatrix>
  </section>
</covarianceSuite>
```

‘array’ container includes support for sparse and/or symmetric arrays
Covariance matrices are stored in a ‘gridded’ container (energy boundaries + axis description + array)

```xml
<covarianceSuite projectile="n" target="Pu239" version="GND 1.7" xmlns:xlink="http://www.w3.org/1999/xlink">
  <section label="1" id="n + Pu239 [total fission] [nuar]" nativeData="covarianceMatrix">
    <rowData xlink:href="/reactionSuite/reaction[@label='45']/.../multiplicity" ENDF_MFMT="35,18"/>
    <covarianceMatrix type="relative">
      <gridded dimension="2">
        <axes>
          <axis index="2" label="row_energy_bounds" unit="eV" gridStyle="boundaries">
            <values length="11">1e-5 1e+5 1e+6 2e+6 6e+6 1e+7 1.4e+7 1.6e+7 1.8e+7 2e+7</values>
          </axis>
          <axis index="1" label="column_energy_bounds" unit="eV" gridStyle="link"/>
          <axis index="0" label="matrix_elements" unit=""/>
        </axes>
        <array shape="10,10" symmetry="lower">
          1.743597e-04
          2.356280e-04 3.184498e-04
          1.378220e-04 1.863129e-04 2.404747e-04 2.648832e-04 2.672193e-04 2.506376e-04 2.174015e-04...
          4.800182e-05 6.488835e-05 8.375597e-05 9.226280e-05 9.309246e-05 8.733193e-05 7.578035e-05...
        </array>
      </gridded></covarianceMatrix></section>
</covarianceSuite>
```

‘array’ container includes support for sparse and/or symmetric arrays

Extra white space added for easy readability, but not required
GND 1.7 overview

- Example: prompt fission neutron multiplicity data with covariance:

```xml
<product name="n" label="n" emissionMode="prompt" >
  <multiplicity>
    <XYs style="eval">
      <axes>...</axes>
      <values length="5452">1e-5 2.8743 ... 2e+7 5.697</values>
    </XYs>
    <uncertainties>
      <uncertainty type="covariance">
        <link xlink:href="/covarianceSuite/section[@label='1']"/>
        <!-- instead of link, could contain the actual matrix -->
      </uncertainty></uncertainties>
  </multiplicity>
</product>
```
GND 1.7 overview

- Example: prompt fission neutron multiplicity data with covariance:

```xml
<product name="n" label="n" emissionMode="prompt" >
  <multiplicity>
    <XYs style="eval">
      <axes>...</axes>
      <values length="5452">1e-5 2.8743 ... 2e+7 5.697</values>
    </XYs>
    <uncertainties>
      <uncertainty type="covariance">
        <link xlink:href="/covarianceSuite/section[@label='1']"/>
      </uncertainty>
    </uncertainties>
  </multiplicity>
</product>
```

Storing uncertainty/covariance together with central values makes association clear.

For other types of covariance (cross terms, covariance for lumped reactions or products), more general method is necessary

<!-- instead of link, could contain the actual matrix -->

```xml
<!-- instead of link, could contain the actual matrix -->
</uncertainty></uncertainties></XYs>

```

```xml
<multiplicity>...</multiplicity></product>
```
Covariances often link different types of data

<table>
<thead>
<tr>
<th></th>
<th>n + U235</th>
<th>n + Au197</th>
</tr>
</thead>
<tbody>
<tr>
<td>(n,elastic)</td>
<td>elastic vs capture</td>
<td>elastic vs fission</td>
</tr>
<tr>
<td>capture vs</td>
<td>(n, gamma)</td>
<td>capture vs fission</td>
</tr>
<tr>
<td>elastic</td>
<td></td>
<td></td>
</tr>
<tr>
<td>fission vs</td>
<td>fission vs capture</td>
<td>(n, fission)</td>
</tr>
<tr>
<td>elastic</td>
<td></td>
<td></td>
</tr>
<tr>
<td>U235 (n, f) vs</td>
<td></td>
<td>U235 (n, f) vs Au197 (n, gamma)</td>
</tr>
<tr>
<td>Au197 (n, gamma)</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

Each block is one ‘section’
GND <covarianceSuite> organizes covariances by section, handles cross terms, lumped sums, etc.

- Links (using xLink syntax) are used to associate rows/columns of each covariance matrix with relevant data.

- If a covariance applies to a sum over reactions (or products), the sum is explicitly defined in the covarianceSuite.

- Resonance parameter covariances (MF32) are similar to others, except matrix elements correspond to parameters instead of energy ranges.
Translation to GND can help clarify data and reveal possible problems:

Sample covariance data (from ENDF-VII.1 O16):

<table>
<thead>
<tr>
<th></th>
<th></th>
<th></th>
<th></th>
<th></th>
<th></th>
<th></th>
<th></th>
<th></th>
<th>182533</th>
<th>4</th>
</tr>
</thead>
<tbody>
<tr>
<td>8.016000+3</td>
<td>1.585751+1</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>1</td>
<td></td>
<td>0</td>
<td>82533</td>
<td>4</td>
</tr>
<tr>
<td>0.000000+0</td>
<td>0.000000+0</td>
<td>0</td>
<td>4</td>
<td>1</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td>82533</td>
<td>4</td>
</tr>
<tr>
<td>0.000000+0</td>
<td>0.000000+0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td>82533</td>
<td>4</td>
</tr>
<tr>
<td>1.000000-5</td>
<td>3.000000+7</td>
<td>0</td>
<td>0</td>
<td>34</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td>1782533</td>
<td>4</td>
</tr>
<tr>
<td>1.000000+0</td>
<td>1.000000+0-1.000000+0</td>
<td>2.000000+0-1.000000+0</td>
<td>1.600000+1</td>
<td>82533</td>
<td>4</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>-1.000000+0</td>
<td>2.200000+1-1.000000+0</td>
<td>2.300000+1-1.000000+0</td>
<td>2.800000+1</td>
<td>82533</td>
<td>4</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>-1.000000+0</td>
<td>3.200000+1-1.000000+0</td>
<td>4.100000+1-1.000000+0</td>
<td>4.400000+1</td>
<td>82533</td>
<td>4</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>-1.000000+0</td>
<td>4.500000+1-1.000000+0</td>
<td>1.020000+2-1.000000+0</td>
<td>1.030000+2</td>
<td>82533</td>
<td>4</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>-1.000000+0</td>
<td>1.040000+2-1.000000+0</td>
<td>1.050000+2-1.000000+0</td>
<td>1.070000+2</td>
<td>82533</td>
<td>4</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>-1.000000+0</td>
<td>1.080000+2-1.000000+0</td>
<td>1.120000+2</td>
<td>82533</td>
<td>4</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>0.000000+0</td>
<td>0.000000+0</td>
<td>1</td>
<td>5</td>
<td>6</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td>382533</td>
<td>4</td>
</tr>
<tr>
<td>1.000000-5</td>
<td>6.430885+6</td>
<td>1.500000+8</td>
<td>0.000000+0</td>
<td>0.000000+0</td>
<td>0.000000+0</td>
<td>82533</td>
<td>4</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>0.000000+0</td>
<td>0.000000+0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td>082533</td>
<td>0</td>
</tr>
</tbody>
</table>
Translation to GND can help clarify data and reveal possible problems:

Sample covariance data (from ENDF-VII.1 O16):

```
<section label="2" id="(z,n)"
  <rowData xlink:href="/reactionSuite/summedReaction[@label='62']/crossSection" ENDF_MFMT="33,4"/>
  <mixed>
    <sum index="0" lowerBound="1e-5 eV" upperBound="3e7 eV"
      <!-- The matrix for this reaction equals the weighted sum of the following matrices: -->
      <summand href="/covarianceSuite/section[@label='0']" coefficient="1.0" ENDF_MFMT="33,1"/>
      <summand href="/covarianceSuite/section[@label='1']" coefficient="-1.0" ENDF_MFMT="33,2"/>
      ...
      <summand href="/covarianceSuite/section[@label='18']" coefficient="-1.0" ENDF_MFMT="33,112"/>
    </sum>
    <covarianceMatrix index="1" type="relative">
      <gridded dimension="2">
        <axes>
          <axis index="2" label="row_energy_bounds" unit="eV" gridStyle="bounds">
            <values length="3">
              1e-5 6430885 1.5e8
            </values>
          </axis>
          <axis index="1" label="column_energy_bounds" gridStyle="link">
            ...
          </axis>
          <axis index="0" label="matrix_elements" unit=""/>
        </axes>
        <array shape="2,2" symmetry="lower">
          0.0
          0.0 0.0
        </array>
      </gridded></covarianceMatrix></mixed></section>
```

Why is this section present?
Moving beyond ENDF-6, what other options for storing covariances will be most useful?

- Use asymmetric uncertainties or non-normal distributions. Example: cross section near threshold.
Moving beyond ENDF-6, what other options for storing covariances will be most useful?

- Compress covariance matrix by only storing principal eigenvalues/vectors
- First few principal components typically dominate the matrix
- In this example (Pu239 PFNS covariance), 4 largest eigenvalues + corresponding vectors are sufficient to reconstruct the full matrix to ENDF precision.
Moving beyond ENDF-6, what other options for storing covariances will be most useful?

- Thermal neutron scattering (thanks to J. Holmes and A. Hawari for their suggestions):
  - $S(\alpha,\beta)$ covariances are high dimensional: $\alpha_i$ vs $\alpha_j$ vs $\beta_k$ vs $\beta_l$ vs $T$. Potentially makes for huge matrices.
  - Not all $\alpha,\beta$ are equal: small $S(\alpha\beta)$ (usually associated with large $\alpha/\beta$) have less impact on results, covariances can be stored on coarser grid.
  - Decompose 5-dimensional array, only use finer grid where needed (where $S(\alpha\beta)$ is large).
Decomposing $S(ab)$ covariance into sub-arrays (pretend original is 3D):

- Use N-D array container for each sub-section (includes support for sparse / symmetric arrays)
GND 1.7 overview

- Central values in GND are organized inside a `<reactionSuite>`:

```xml
<reactionSuite projectile="..." target="..." formatVersion="..." ...
  <styles> e.g. ‘evaluated’ or ‘processed’ </styles>
  <documentations> support ascii, html, etc. </documentations>
  <particles> ground state, levels, gammas ... </particles>
  <resonances>
    <resolved>...</resolved>
    <unresolved>...</unresolved></resonances>
... followed by a list of `<reaction>` elements
</reactionSuite>
```
GND 1.7 covarianceSuite overview

<covarianceSuite projectile="..." target="..." formatVersion="...">

  <styles ... > evaluated, processed, etc. </styles>

  <externalReactions> for cross-material covars </externalReactions>

  <section label="..." id="..." nativeData="covarianceMatrix">
    <rowData xlink="..."/>

    <columnData xlink="..."/>

    <covarianceMatrix> ... </covarianceMatrix></section>

  <section label="..." id="...">...</section>

  <section label="..." id="...">...</section>

  <section label="..." id="...">...</section>

  ...

</covarianceSuite>