Uncertainties and covariances in SG38 and GND-1.7

Joint meeting of WPEC subgroups 38,39 and 40

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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:

```
<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 comment

GND 1.7 overview

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

```
<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>
```

<uncertainties> element can appear at several points

color code:

element attribute comment

GND 1.7 overview

- Example: prompt fission neutron multiplicity data with covariance:

```
<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>...</multiplicity></product>
```

GND 1.7 overview

- Example: prompt fission neutron multiplicity data with covariance:

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

```
<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 1.4.+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
          3.039931e-04  4.108886e-04  5.302406e-04
          3.347426e-04  4.524720e-04  5.839602e-04  6.431584e-04
          3.376183e-04  4.563926e-04  5.890303e-04  6.487303e-04  6.544328e-04
          3.165935e-04  4.279883e-04  5.523777e-04  6.084044e-04  6.137411e-04  5.755823e-04
          2.745613e-04  3.711586e-04  4.790528e-04  5.276573e-04  5.322913e-04  4.992121e-04  4.329712e-04
          2.141380e-04  2.894741e-04  3.736303e-04  4.115408e-04  4.151704e-04  3.893697e-04  3.377302e-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_MF
  <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 1.4.+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
       3.039931e-04  4.108886e-04  5.302406e-04
       3.347426e-04  4.524720e-04  5.839602e-04  6.431584e-04
       3.376183e-04  4.563926e-04  5.890303e-04  6.487303e-04  6.544328e-04
       3.165935e-04  4.279883e-04  5.523777e-04  6.084044e-04  6.137411e-04  5.755823e-04
       2.745613e-04  3.711586e-04  4.790528e-04  5.276573e-04  5.322913e-04  4.992121e-04  4.329712e-04
       2.141380e-04  2.894741e-04  3.736303e-04  4.115408e-04  4.151704e-04  3.893697e-04  3.377302e-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

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_MF
    <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 1.4.+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
          3.039931e-04  4.108886e-04  5.302406e-04
          3.347426e-04  4.524720e-04  5.839602e-04  6.431584e-04
          3.376183e-04  4.563926e-04  5.890303e-04  6.487303e-04  6.544328e-04
          3.165935e-04  4.279883e-04  5.523777e-04  6.084044e-04  6.137411e-04  5.755823e-04
          2.745613e-04  3.711586e-04  4.790528e-04  5.276573e-04  5.322913e-04  4.992121e-04  4.329712e-04
          2.141380e-04  2.894741e-04  3.736303e-04  4.115408e-04  4.151704e-04  3.893697e-04  3.377302e-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

- Example: prompt fission neutron multiplicity data with covariance:

```
<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>...</multiplicity></product>
```

GND 1.7 overview

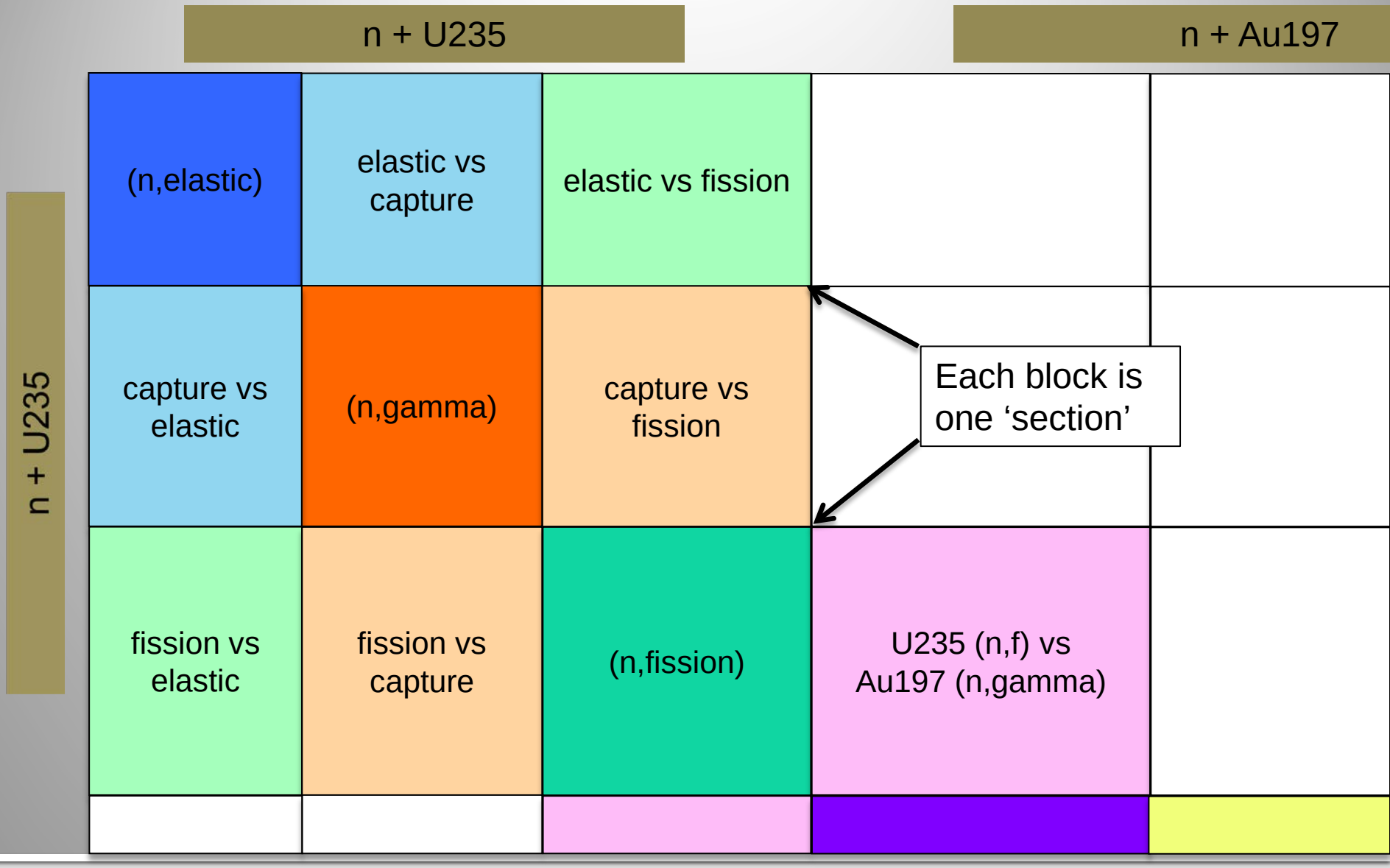
- Example: prompt fission neutron multiplicity data with covariance:

```
<product name="n" label="n" emissionMode="prompt" >
  <multiplicity>
    <XYs style="eval">
      <axes>...</axes>
      <values length="5452">1e
      <uncertainties>
        <uncertainty type="cova
          <link xlink:href="/cova
          <!-- instead of link, could contain the actual matrix -->
        </uncertainty></uncertainties></XYs>
  <multiplicity>...</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

Covariances often link different types of data



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):

```
 8.016000+3 1.585751+1          0          0          0          1 82533  4
 0.000000+0 0.000000+0          0          4          1          1 82533  4
 0.000000+0 0.000000+0          0          0          0          0 82533  4
 1.000000-5 3.000000+7          0          0         34         17 82533  4
 1.000000+0 1.000000+0-1.000000+0 2.000000+0-1.000000+0 1.600000+1 82533  4
-1.000000+0 2.200000+1-1.000000+0 2.300000+1-1.000000+0 2.800000+1 82533  4
-1.000000+0 3.200000+1-1.000000+0 4.100000+1-1.000000+0 4.400000+1 82533  4
-1.000000+0 4.500000+1-1.000000+0 1.020000+2-1.000000+0 1.030000+2 82533  4
-1.000000+0 1.040000+2-1.000000+0 1.050000+2-1.000000+0 1.070000+2 82533  4
-1.000000+0 1.080000+2-1.000000+0 1.120000+2                       82533  4
 0.000000+0 0.000000+0          1          5          6          3 82533  4
 1.000000-5 6.430885+6 1.500000+8 0.000000+0 0.000000+0 0.000000+0 82533  4
 0.000000+0 0.000000+0          0          0          0          0 82533  0
```

Translation to GND can help clarify data and reveal possible problems:

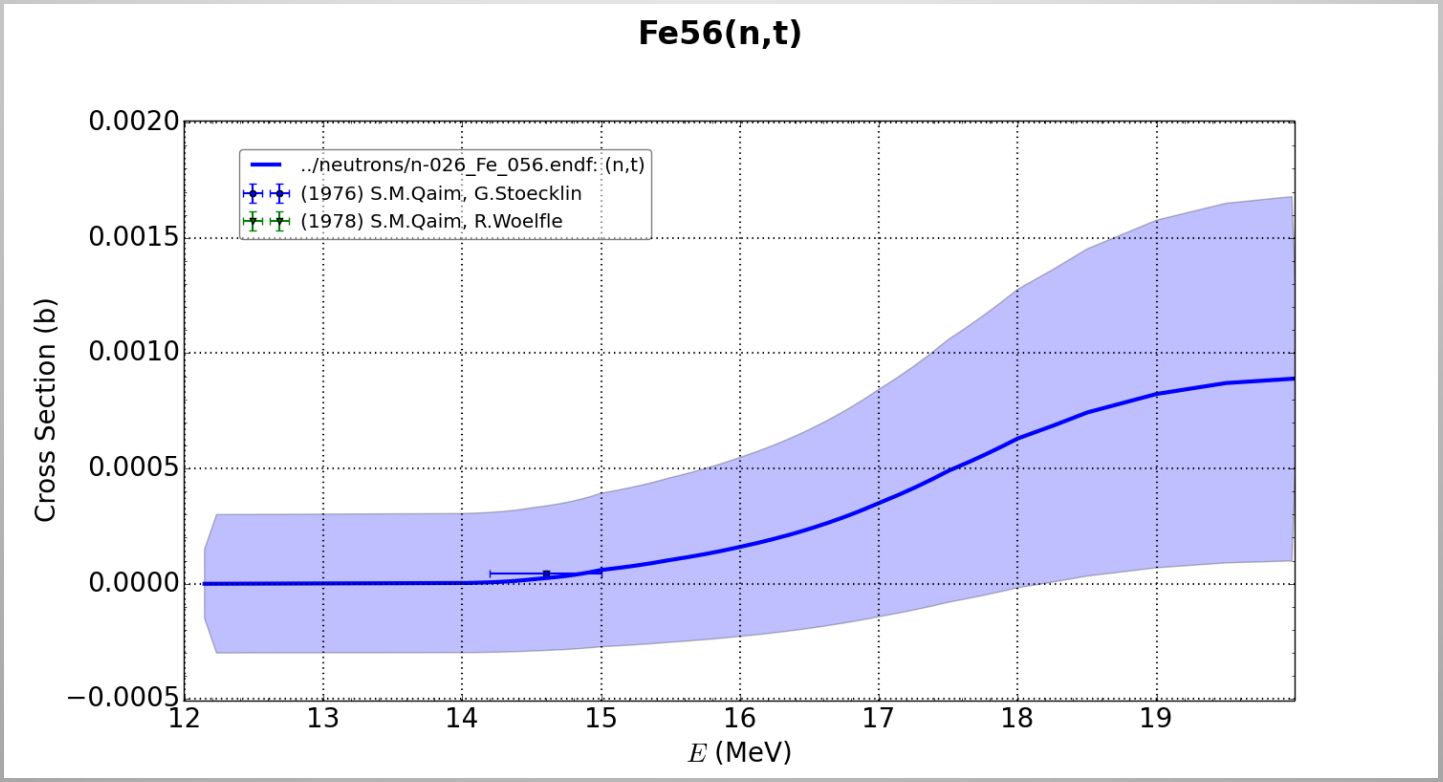
Sample covariance data (from ENDF-VII.1 O16):

```
<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?

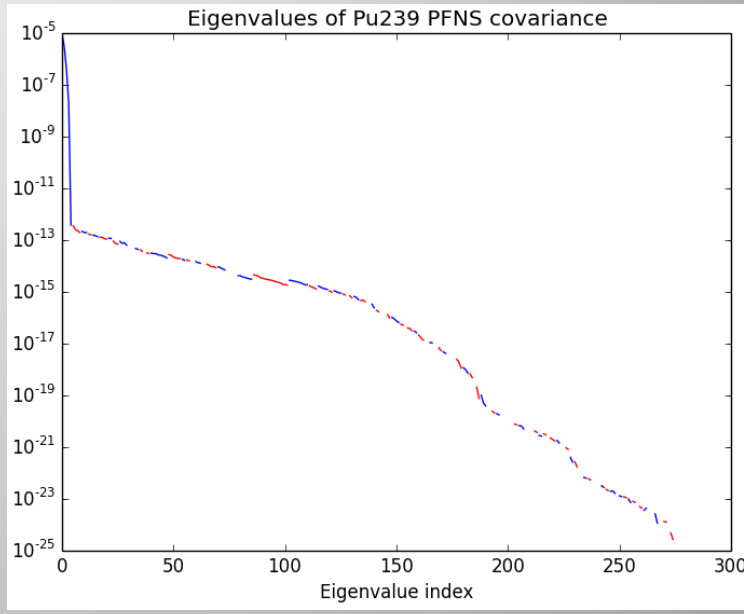
Moving beyond ENDF-6, what other options for storing covariances will be most useful?

- 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?

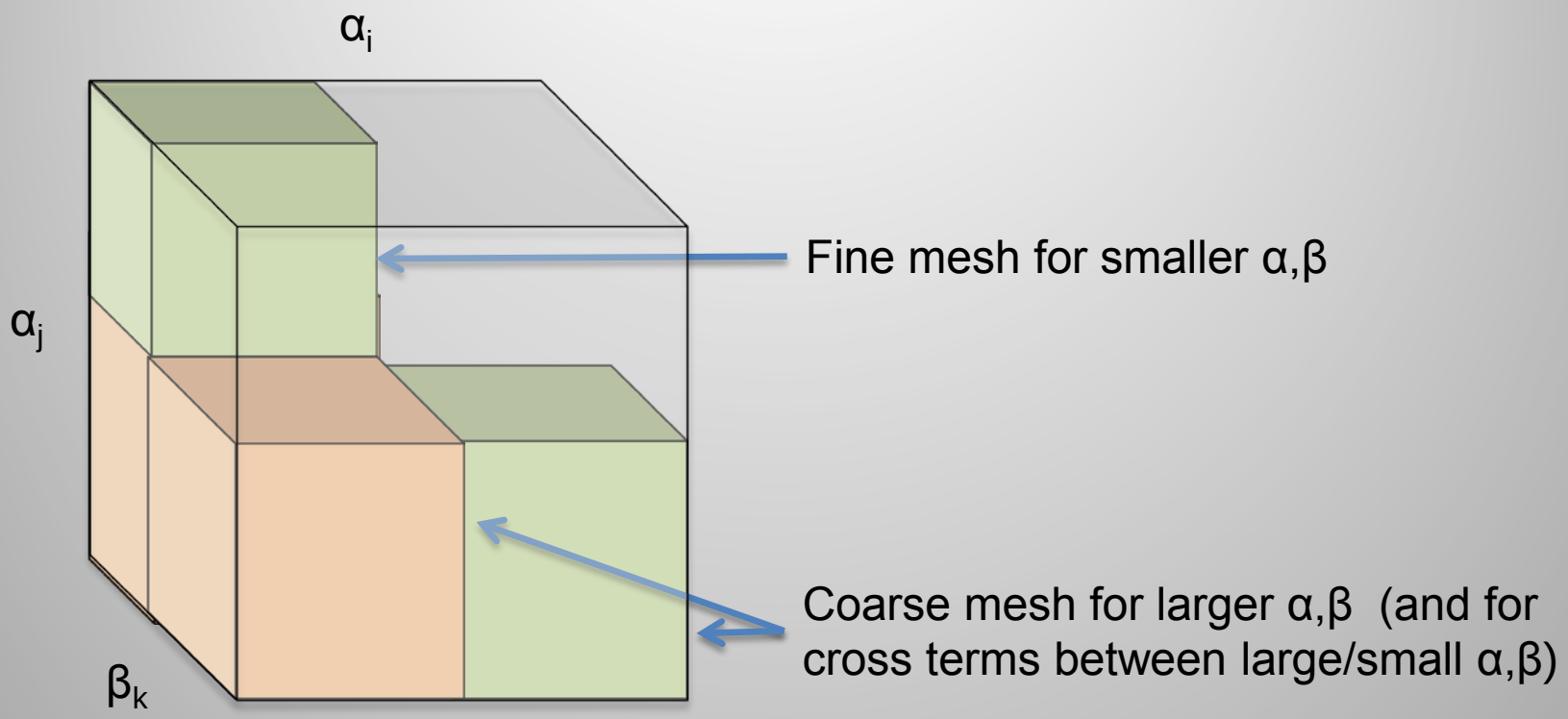
- Compress covariance matrix by only storing principal eigenvalues/vectors
- First few principal components typically dominate the matrix
- In this example (Pu239 PFNS covariance), 4 largest eigenvalues + corresponding vectors are sufficient to reconstruct the full matrix to ENDF precision.



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(α,β) covariances are high dimensional: α_i vs α_j vs β_k vs β_l vs T. Potentially makes for huge matrices
  - Not all α,β are equal: small S(αβ) (usually associated with large α/β) have less impact on results, covariances can be stored on coarser grid
  - Decompose 5-dimensional array, only use finer grid where needed (where S(αβ) 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)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GND 1.7 overview

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

<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>

color code:

element attribute comment

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>
    ...
</covarianceSuite>
```