GNDS 1.9 Covariance Format + proposed changes

2019 CSEWG Covariance session

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Covariances are included in the first official GNDS specification (GNDS-1.9)

- GNDS-1.9 specifications to be published soon by NEA.
  - Draft version available at https://www.oecd-nea.org/science/wpec/gnds/
- Supports *most* types of covariance data found in ENDF-6 manual, *all* types found in ENDF/B-VII.1 and ENDF/B-VIII
- I will briefly describe GNDS-1.9 covariances, and present a draft proposal for new covariances in the next version of GNDS

GNDS covariance sections fall into two general categories:

- Parameter covariances (like ENDF MF=32)
  - Consisting of an NxN matrix along with links to N parameters
  - All co-variant parameters are included in the matrix

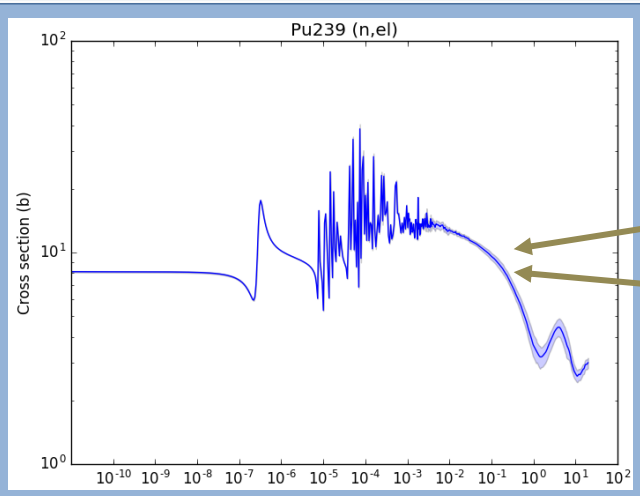
- Everything else (MF=31,33,34,35,40)
  - Consist of links to the row (and optionally column) data, a list of energy boundaries along each axis, and a covariance matrix or recipe for deriving a covariance matrix

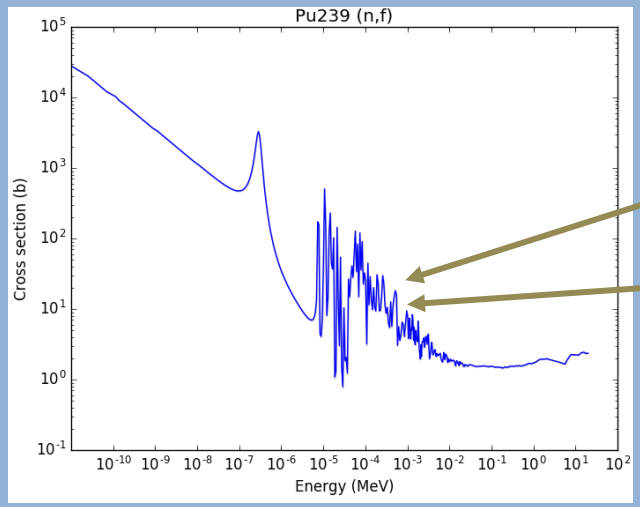
Parameter covariances used for RRR and for some polynomial expansions (e.g. for fission energy release)

- Parameter covariances have two parts
  - One or more links pointing to N co-variant parameters
    - A single link can point to multiple parameters inside a table
  - An NxN matrix

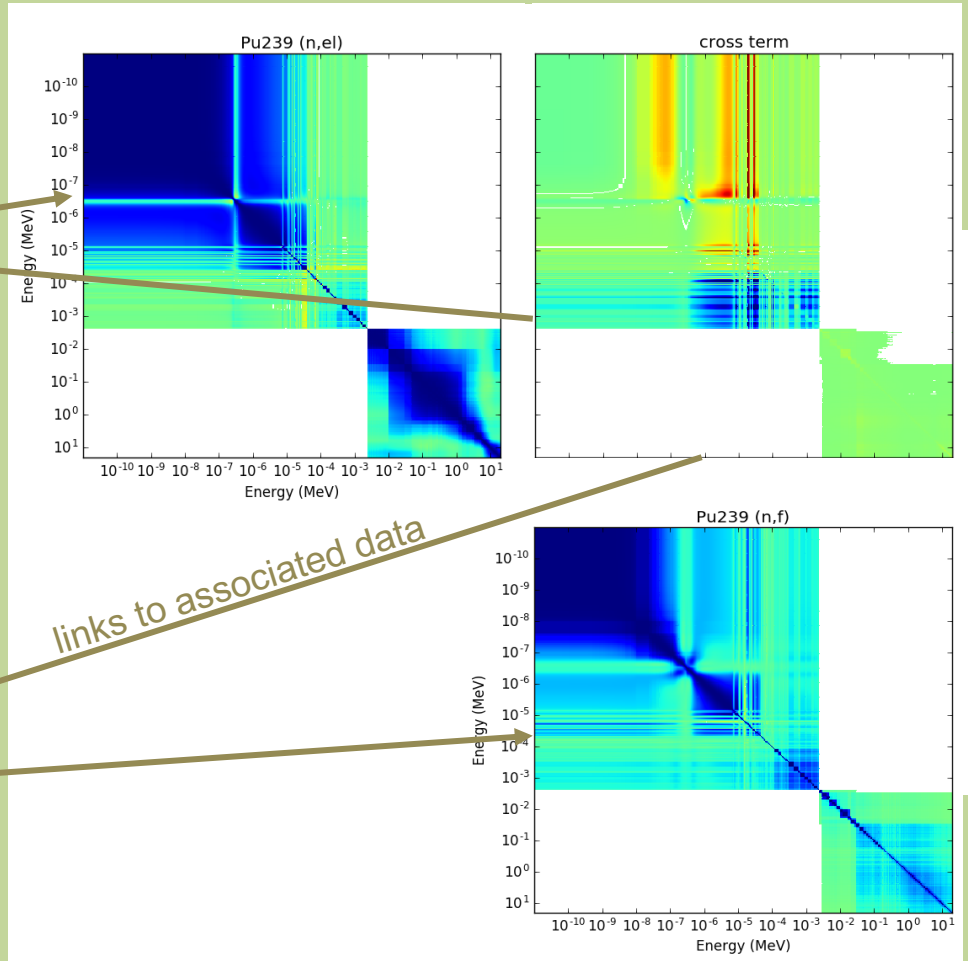
```
<parameterCovarianceMatrix label="eval" type="absolute">
  <parameters>
    <parameterLink label="0" href=".../spinGroup[@label='0']/resonanceParameters/table" nParameters="99"/>
    <parameterLink label="1" href=".../spinGroup[@label='1']/resonanceParameters/table" nParameters="108" matrixStartIndex="99"/>
    ...
    <parameterLink label="6" href=".../spinGroup[@label='6']/resonanceParameters/table" nParameters="42" matrixStartIndex="426"/>
    <parameterLink label="7" href=".../spinGroup[@label='7']/resonanceParameters/table" nParameters="93" matrixStartIndex="468"/>
  </parameters>
  <array shape="561,561" symmetry="lower">
    <values> ... (list of 157641 values) ... </values>
  </array>
</parameterCovarianceMatrix>
```

GNDS uses links to associate data across different files or different sections of a file





reactionSuite



covarianceSuite

‘Standard’ covariances used for cross section, nubar, outgoing spectra and URR parameters

- Full covariance matrix is decomposed into blocks or ‘sections’.
- Blocks along the diagonal relate to a single quantity:

```
<section label="2n + Mn54 + photon">
  <rowData ENDF_MFMT="33,16" href="../reaction[@label='2n + Mn54 + photon']/crossSection/XYs1d[@label='eval']"/>
  <covarianceMatrix label="eval" type="relative">
    <gridded2d>
      <axes>
        <grid index="2" label="row_energy_bounds" unit="eV" style="boundaries">
          <values>... define energy bounds for each matrix element ...</values></grid>
        <grid index="1" label="column_energy_bounds" unit="eV" style="link">
          <link href="../../grid[@index='2']/values"/></grid>
        <axis index="0" label="matrix_elements" unit=""/></axes>
      <array shape="9,9" symmetry="lower">
        <values>... (list of 45 values) ...</values>
      </array>
    </gridded2d>
  </covarianceMatrix>
</section>
```

‘array’ container may use diagonal, symmetric or sparse storage to reduce size

‘Standard’ covariances used for cross section, nubar, outgoing spectra and URR parameters

- Full covariance matrix is decomposed into blocks or ‘sections’.
- Off-diagonal blocks are cross-terms relating two different quantities:

```
<section label="2n + Mn54 + photon vs. 3n + Mn53 + photon" crossTerm="true">
  <rowData ENDF_MFMT="33,16" href=".../reaction[@label='2n + Mn54 + photon']/crossSection/XYs1d[@label='eval']"/>
  <columnData ENDF_MFMT="33,17" href=".../reaction[@label='3n + Mn53 + photon']/crossSection/XYs1d[@label='eval']"/>
  <covarianceMatrix label="eval" type="relative">
    <gridded2d>
      <axes>
        <grid index="2" label="row_energy_bounds" unit="eV" style="boundaries">
          <values>8971600 ... 6e7</values></grid>
        <grid index="1" label="column_energy_bounds" unit="eV" style="boundaries">
          <values>1.4219e7 ... 6e7</values></grid>
        <axis index="0" label="matrix_elements" unit=""/></axes>
      <array shape="9,7">
        <values>... (list of 63 values) ...</values>
      </array>
    </gridded2d>
  </covarianceMatrix>
</section>
```

Covariances need not be stored as a single matrix

- A section may consist of multiple independent matrices that should be summed together
  - Like multiple NI sub-subsections in ENDF-6
- May be computed as the sum of other sections
  - like NC, LTY=0-4 sections in ENDF-6
- May include ‘short-range self-scaling’ variance terms
  - Like NI sub-subsection with LB=8 or 9 in ENDF-6

Sections are a flexible way to handle covariances and cross terms

- rowData/columnData links can point to any type of data in GNDS file
  - Makes covariance between cross-section and nubar simple: rowData points to the cross section, columnData points to nubar

- Metadata on rowData and columnData support higher-dimensional covariances
  - PFNS covariance matrices are applicable over a range of incident energies. The incident energy range is specified in the rowData
  - Similar strategy may be sufficient to support covariances on S(α,β)

```
<section label="m(E)*n + photon [total fission] [spectrum] energy range 0">
  <rowData ENDF_MFMT="35,18" domainMin="1e-05" domainMax="500000.0" domainUnit="eV"
           href="$reactions#/.../fission/.../distribution/uncorrelated[@label='eval']/energy"/>
  ...
```

Proposal for next GNDS version: support storing 'sandwichProduct' covariances

- Covariance matrices can often be decomposed into a matrix product:

$$\mathrm{cov}x_{ij} = \sum_k (\vec{v}_k)_i \lambda_k (\vec{v}_k)_j$$

- v_k and λ may be much smaller than the full covariance.

- This type of matrix representation addresses several needs:
  - Storing only principal eigenvalues / eigenvectors
  - Storing a parameter covariance along with a sensitivity matrix

- Despite several discussions, this format was missing from GNDS-1.9 specifications

Tentative sandwichProduct example:

- λ becomes ‘innerCovariance’
- Left and right vectors become <rowVectors> and <columnVectors>
  - For symmetric arrays, columnVectors = transpose of rowVectors

```
<sandwichProduct label="eval" type="absolute">
  <axes>...</axes>
  <innerCovariance>
    <array shape="10,10" compression="diagonal">...</array>
  </innerCovariance>
  <rowVectors>
    <array shape="275,10">...</array>
  </rowVectors>
  <columnVectors>   <!-- for non-symmetric matrices only -->
    <array shape="10,275">...</array>
  </columnVectors>
</sandwichProduct>
```

Summary

- GNDS-1.9 defines flexible containers for storing covariances
  - Requested features like S(α,β) and fission product yield covariances appear to fit neatly into existing GNDS containers
- Future extensions to GNDS should give evaluators more flexibility to express covariances.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