Options for storing TSL covariances in GNDS

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GNDS handles nearly all data appearing in ENDF-6 evaluations, now time to focus on adding new capabilities, such as TSL covariances.

- Latest release (GNDS-1.9) handles thermal scattering law data, but data organization may still change (discussed in SG-42 and EG-GNDS meetings).

  - Adding covariances should be straight-forward, but we need feedback from TSL experts before proceeding.

  - Here I show some tentative proposals for storing these covariances

First a brief review of typical covariances in GNDS:

- reaction
  - crossSection

One cross section may have multiple representations, or 'styles'. Each style may have corresponding covariance

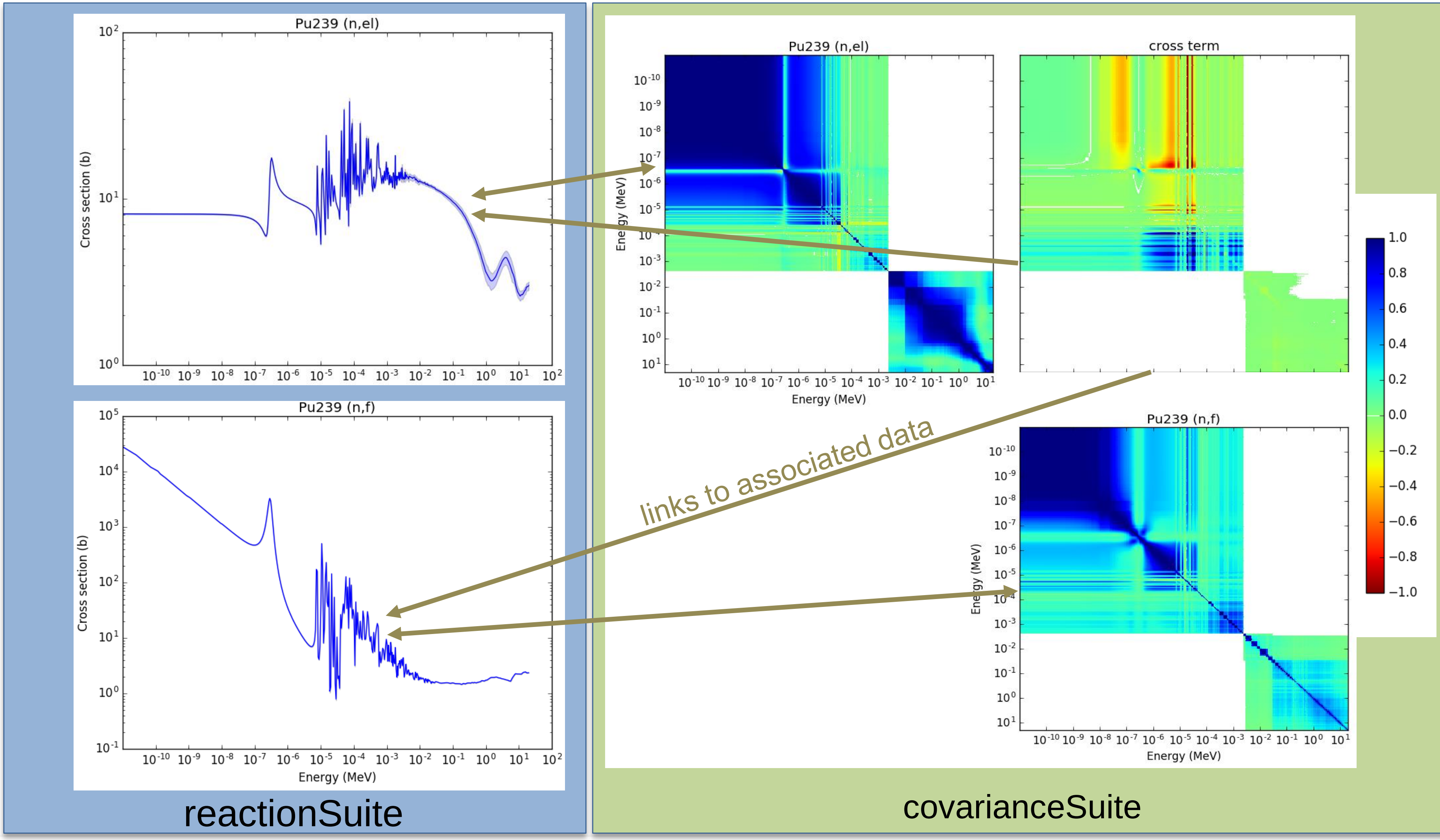
— resonancesWithBackground label="evaluated"
  – link to resonance parameters
  – background cross section interpolation="log-log"
    • values
    • covariance

— XYs1d label="crossSectionReconstructed" interpolation="lin-lin"
  – values
  – covariance

— gridded1d label="multigroup" interpolation="flat"
  – values
  – covariance

May be full covariance, or may be a link to a matrix in the covarianceSuite

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



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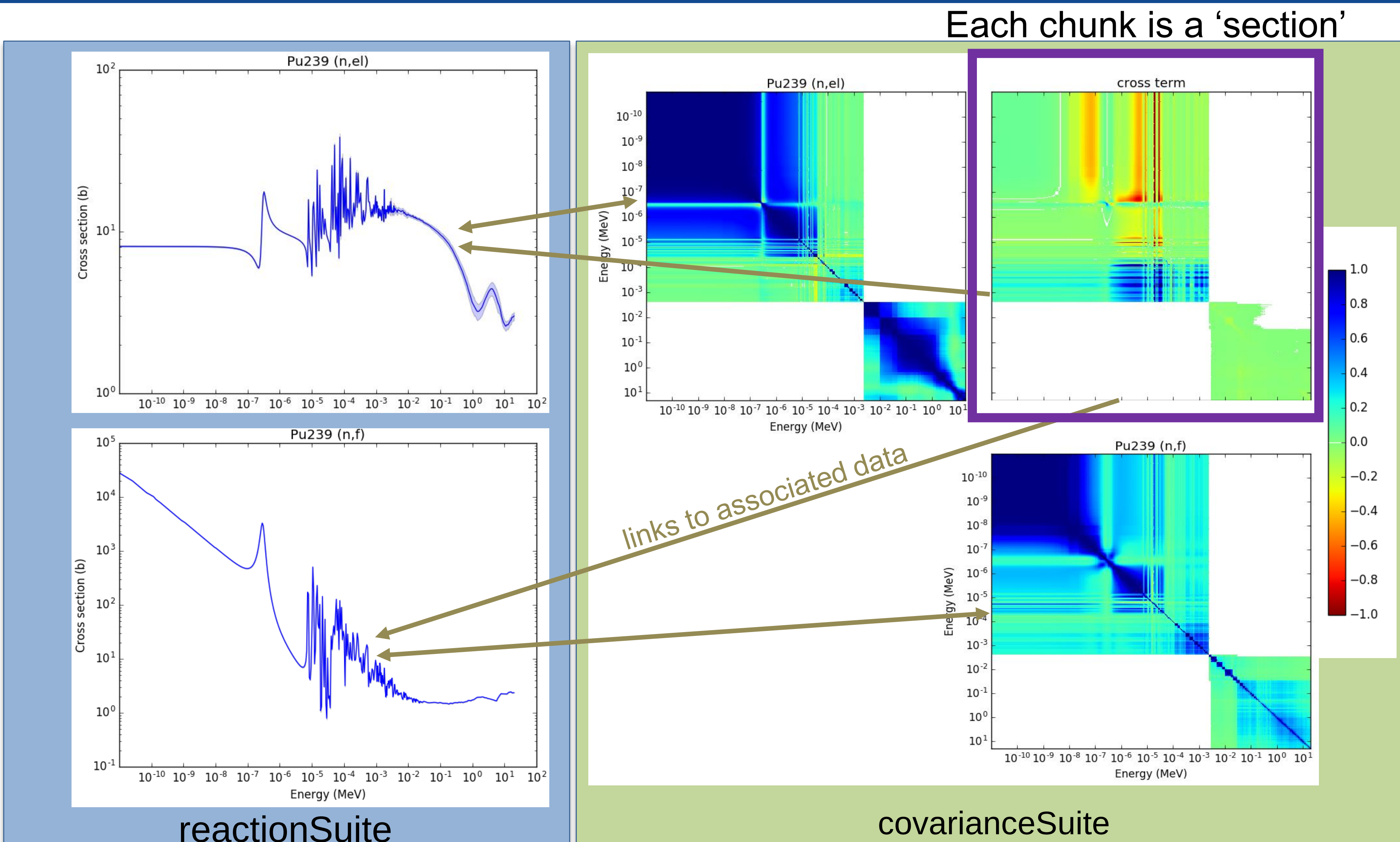

Example of a covariance stored in XML

```xml
<section label="2n + O15 + photon">
  <rowData ENDF_MFMT="33,16" href="$reactions#/reactionSuite/reactions/
       reaction[@label="…"]/crossSection/XYs1d[@label='eval']"/>
  <covarianceMatrix label="eval" type="relative">
    <gridded2d>
      <axes>
        <grid index="2" label="row_energy_bounds" unit="eV" style="boundaries">
          <values>1e-5 16651600 1.7e7 2e7 3e7 1.5e8</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="5,5" symmetry="lower">
        <values>0 0 0.25 0 0 0.0625 0 0 0.025 4e-2 0 0 0 0 0</values>
      </array>
    </gridded2d>
  </covarianceMatrix>
</section>
```

Like other cross sections, thermal scattering data (and covariances) may have multiple forms

- Original form: input parameters to a molecular dynamics (or similar) code that produces phonon spectrum
  - No single code or model covers all types of TSL evaluations?
- Second form: input to LEAPR (or similar)
- Partially processed: $S_{\alpha\beta}(T)$ for inelastic, cumulative S factor for coherent elastic, etc.
- Further processed: cross sections / outgoing energy and angle distributions, possibly grouped and/or converted to transfer matrices

  - Each form potentially needs associated covariances

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Covariances for input parameters

- Future evaluations could store TSL as model parameters (i.e. inputs to LEAPR or similar)

Table 1
LEAPR parameters for H in H_2O at 294 K and 574 K established by Mattes and Keinert (2005).

Parameters		T = 294 K	T = 574 K
Diffusion constant	c	0.0	0.0
Energy interval (meV)	δ	2.542	2.542
First oscillator energy (meV)	E_1	205.0	205.0
Second oscillator energy (meV)	E_2	436.0	436.0
Continuous spectrum weight	w_c	0.4891	0.4773
Translational weight	w_t	0.0217	0.0454
First oscillator weight	w_1	0.1630	0.1591
Second oscillator weight	w_2	0.3261	0.3182
Free scattering cross section (barn)	σ_s	20.478	20.478

Simplified model for continuum

Noguere et. al., Annals Nuc. En. 104 (2017)

Covariances for input parameters

- LEAPR parameter table represented in GNDS:

```
<thermalScattering material="...">
  <styles>...</styles>
  <documentation>...</documentation>
  <incoherentInelastic>
    <scatteringAtoms>...</scatteringAtoms>
    <LEAPR_model label="eval">
      <table rows="2" columns="10">
        <columnHeaders>
          <column index="0" name="Temperature" unit="K"/>
          <column index="1" name="Diffusion constant" unit=""/>
          <column index="2" name="Energy interval" unit="meV"/>
          <column index="3" name="First oscillator energy" unit="meV"/>
          ...
          <column index="9" name="Free scattering cross section" unit="b"/>
        </columnHeaders>
        <data>
          294   0   2.542   205.0   436.0   0.4891    0.0217    0.1630    0.3261    20.478
          574   0   2.542   205.0   436.0   0.4773    0.0454    0.1591    0.3182    20.478
        </data>
      </table>
    </LEAPR_model>
  </incoherentInelastic>
</thermalScattering>
```

Covariances for input parameters

- Corresponding parameter covariance:

```
<parameterCovariances>
  <parameterCovariance label="LEAPR inputs">
    <rowData href="/thermalScattering/incoherentInelastic/LEAPR_model[@label='eval']"/>
    <parameterCovarianceMatrix label="eval" type="absolute">
      <parameters>
        <parameterLink label="params"
                       href="/thermalScattering/incoherentInelastic/LEAPR_model[@label='eval']/table"
                       nParameters="20"/>
      </parameters>
      <array shape="20,20" symmetry="lower">
        <values>...</values>
      </array>
    </parameterCovarianceMatrix>
  </parameterCovariance>
</parameterCovariances>
```

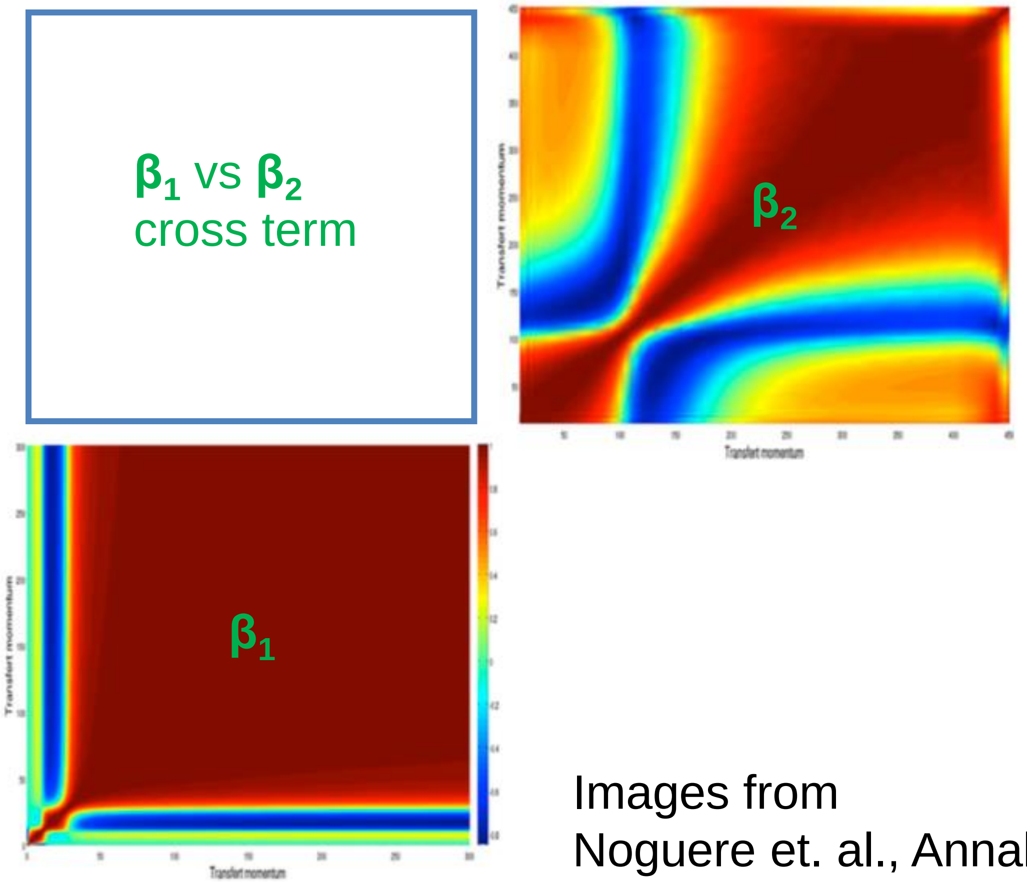
  - Matrix contains rows/columns of all zero for parameters that were not varied in the fit (e.g. temperature)

Covariances for $S_{\alpha\beta}$:

- S is a function of α,β, and temperature
  - For now neglect cross-terms between different material temperatures
  - Problem then is to store the covariance for a 2-dimensional function. In order to capture correlations between all α_1, α_2, β_1, β_2 we need a 4-dimensional covariance
    - Can be decomposed into multiple 2-d matrices, i.e. one matrix for each combination of β_1, β_2

Most intuitive option could be to decompose $S_{\alpha,\beta}$ covariance into sub-arrays

- Could store cov(α_1, α_2) for a range of β (or vice versa), with additional cross terms between different β



Images from
Noguere et. al., Annals Nuc. En. 104 (2017)

Decomposing into 2-d sections has advantages / disadvantages

- No need to use the same α grid for each β_1, β_2 combination, could use sparse grids to save space

- But… if same grid is used everywhere, there’s lots of redundancy

One alternative could be to store as a 4-dimensional array*

- Saves space assuming the same α, β grid used for all covariances
- Symmetry rules somewhat more complicated than 2-d matrices:

$$C[\beta_1, \beta_2, \alpha_1, \alpha_2]$$

- Array is symmetric for exchange of β_1 with β_2 or α_1 with α_2, but not β_i with α_i
- For N discrete β values and M discrete α values, full covariance requires M^2N^2 points, symmetric covariance requires N*M * (N*M+1)/2 points

*grows to 6 dimensions if T-dependence is included

Another alternative: covariances (at least in H2O example) appear fairly smooth. What about storing a parameterized form? Or PCA?

- PCA approach does well for prompt fission neutron spectrum, reducing the amount of data stored while preserving matrix properties. Could also be useful for $S_{\alpha\beta}$

Some questions:

- When storing full $S_{\alpha\beta}$ covariance, are the uncertainties in free scattering cross section (and other terms) included, or do they need to be accounted for separately?

- If $S_{\alpha\beta}$ (incoherent inelastic) and cumulative S (coherent elastic) are derived from same phonon spectrum, should they be linked by a cross-covariance?

- What about Debye-Waller or other forms?