Covariances in GND, and feedback on ENDF-VII.1 covariances

CSEWG Covariance session

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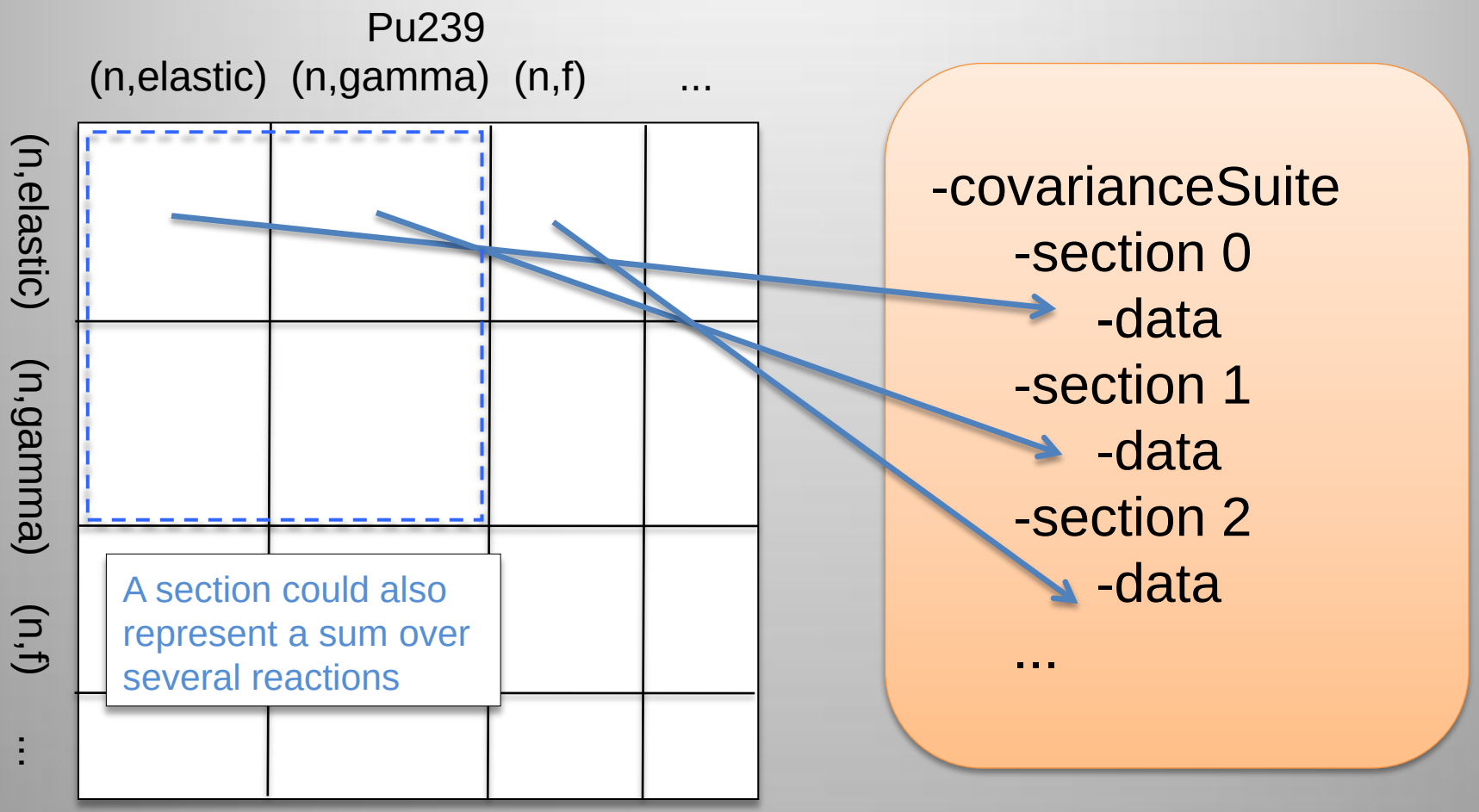
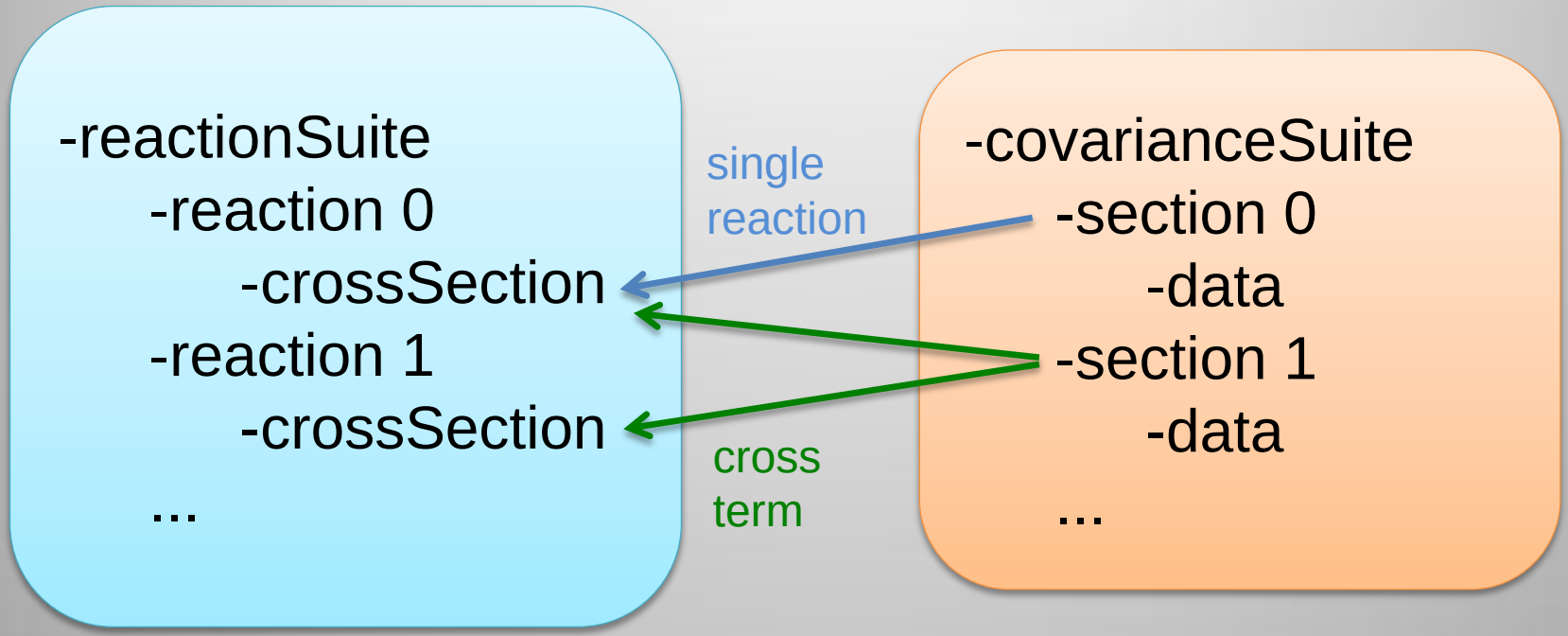
Part I: Overview of covariances in GND:

- In addition to the ‘reactionSuite’, GND maintains a separate ‘covarianceSuite’, with matrices and explicit links pointing back to the reactionSuite
- Advantage: users can skip reading covariances until necessary. Cross-material terms dealt with in consistent fashion
- Disadvantage: keeping covariances separate from other data raises the risk of losing the connection between the two
  - For example, evaluator may revise a cross section but forget to update the covariance

Each section of the covarianceSuite corresponds to a rectangular chunk of the 'full' covariance matrix:



Each section is identified by link(s) to the associated data:



- Need links in the other direction too!

Use ‘xPath’ standard to store links:

- xPath allows linking to a specific point within a file
- For example:

  xlink:href="/reactionSuite/reaction[@label='0']/crossSection”

  xlink:href=“n-025_Mn_055.gnd.xml#/reactionSuite/
  reaction[@label=‘1’]/crossSection”
- xPath was designed for XML, but applies to any hierarchical meta-language

Within each section GND supports several ways of storing a covariance:

- Single covariance matrix
- Sum of multiple matrices
  - each separate matrix generally represents a different uncertainty source
- Weighted sum of other sections
  - for example, if the elastic cross section is defined as “total minus all other channels”, its covariance can be derived by combining these other reactions’ matrices

Currently we support the same covariance options as ENDF-6. Should we support additional options?

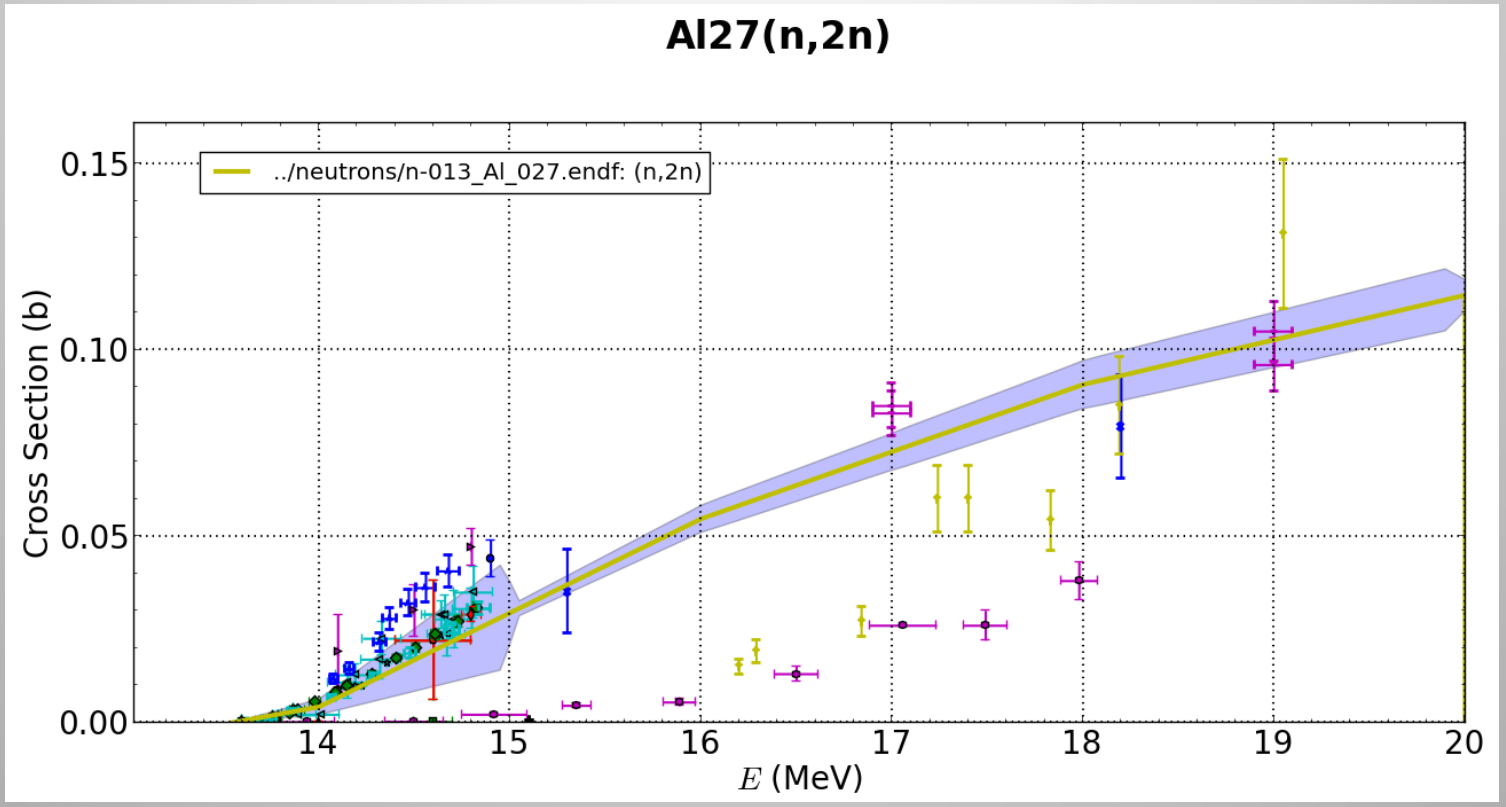
- Covariances for double-differential data (MF=6)
- Covariances between both incident and outgoing energies for energy spectra (e.g. PFNS)
- Expanded options for model parameter covariances
- (Last-minute addition): Log-normal distributions

Part II: complaints about ENDF-VII.1 covariances

- Users are interested in using nuclear data uncertainties as part of UQ studies

- Covariance matrices may have features that make getting realistic samples difficult:
  - Large steps up or down in uncertainty
  - Negative eigenvalues

Al27 (n,2n) is an example of a covariance with large uncertainty near threshold



- Users who try +/- 1 sigma variations are suspicious about shape of the results.

Other common problems:

- Cyclic dependencies: covariance for one MT may be calculated from other MTs.
  - Problem: (total = elastic + ...) ***and*** (elastic = total - ...)
  - This problem appears in Li7, Si28,29,30, Cr50,53, Fe54,56,57, Pb204,206,207,208

- Negative eigenvalues indicate problems with the covariance matrix
  - Many occurrences, although most are small. U235 is the only case worse than -1e-6

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Example of a covarianceMatrix in GND:

- covarianceMatrix, type="relative”
  - axes
    - axis, label="row_energy_bounds”, unit="eV”, length=“51”, interpolation="linear,flat”, length="51”

      ... group boundaries ...

    - axis, label="column_energy_bounds”, unit="eV”, interpolation="linear,flat" mirror_row_energies="true”
    - axis, label="matrix_elements”, unit=””
  - matrix, rows="50”, columns="50”, form="symmetric”

    ... list of (50 * 51)/2 floats ...

Another possible slide:

- This slide still needs work: based on discussion with P. Talou
- What happens if we try to directly sample these matrices? Cholesky decompose and then multiply a random (normally-distributed) vector by the Cholesky L to get a sampled cross section. How reasonable are the results?