Progress on the Development of Thermal Scattering Covariance Formats

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Project Team

- Dr. Vladimir Sobes
  - R&D Staff in Reactor and Nuclear Systems Division at ORNL since 2015
  - Coordinator for NEA WPEC Subgroup 44 on covariance data
  - Nuclear data expert and experienced with SCALE code system

Project Team – Format and Continuous Energy Data

- Prof. Brian Kiedrowski (PI)
  - Assistant Professor at University of Michigan since 2014
  - MCNP developer at LANL from 2010-2014 focused on S/U methods in MCNP
- Aaron G . Tumulak
  - Doctoral student at University of Michigan since 2018
  - Experience writing transport related software at INL and LANL

Project Team – Processing for Multigroup Data

- Prof. Won Sik Yang
  - Professor at University of Michigan since 2017
  - Very experienced reactor physicist, led S/U efforts at ANL (2002 – 2011)
- Hansol Park
  - Postdoc at University of Michigan since 2018
  - Experience in multigroup cross section processing for thermal reactors.

Theory

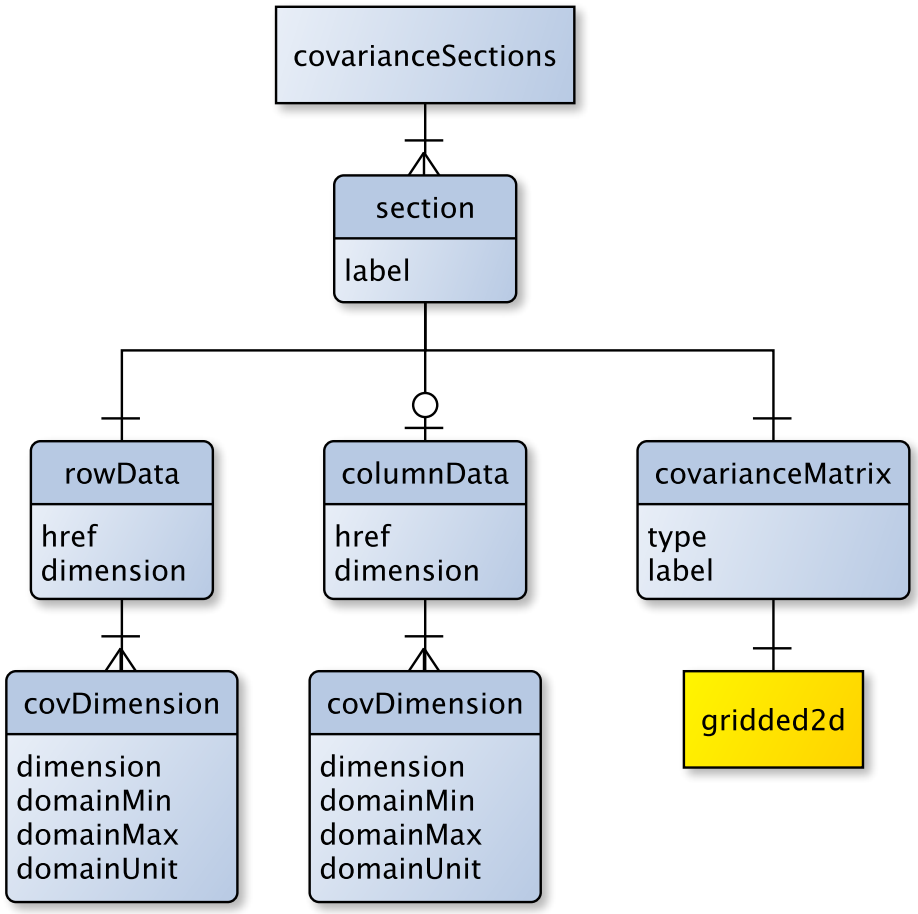
Inelastic scattering cross section for neutrons at thermal energies incident on a system of particles have double differential scattering cross section given by:

$$\sigma(E \to E', \mu) = \frac{\sigma_b}{2k_b T}\sqrt{\frac{E'}{E}}\, e^{-\frac{\beta}{2}} S(\alpha, \beta)$$

$$\alpha = \frac{E' + E - 2\mu\sqrt{EE'}}{Ak_B T}, \qquad \beta = \frac{E' - E}{k_B T}$$

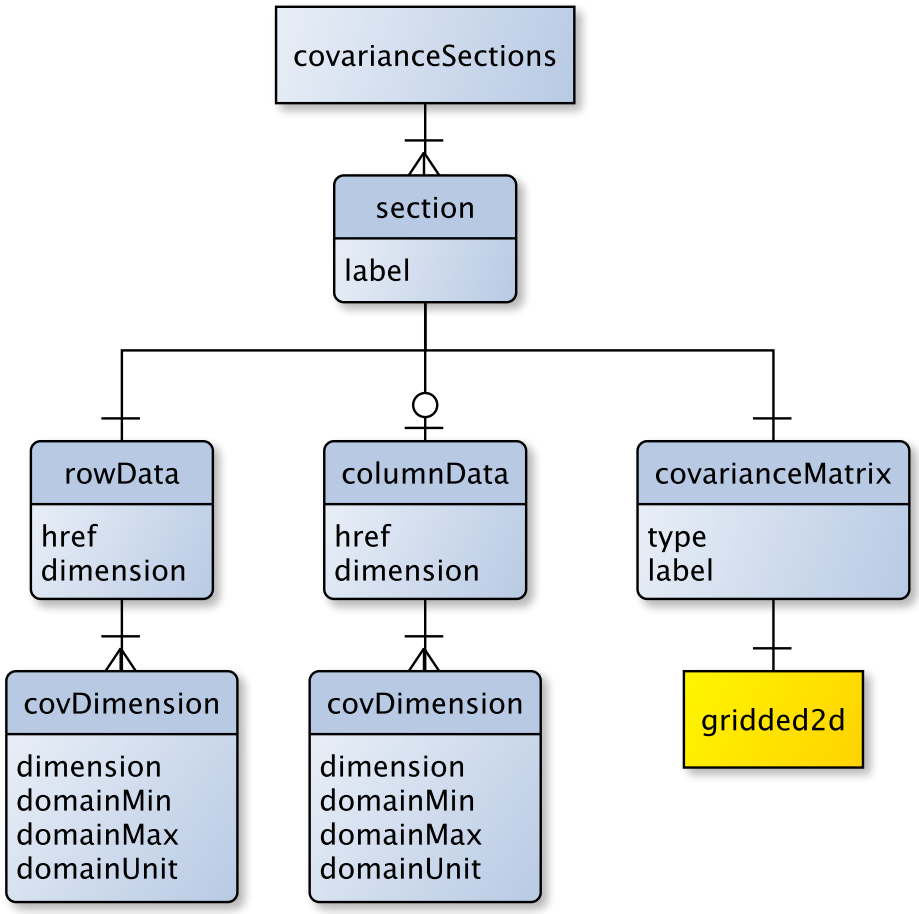
Format Proposal

- As of ENDF-6, there is no format for expressing covariances across two $S(\alpha, \beta)$ values.
- The full covariance matrix is divided into 2D sections.
- rowData (one required): specifies corresponding value for each row of covarianceMatrix
- covDimension (one or many): specifies fixed parameters in covarianceMatrix
- columnData (zero or one): used for cross-covariance sections



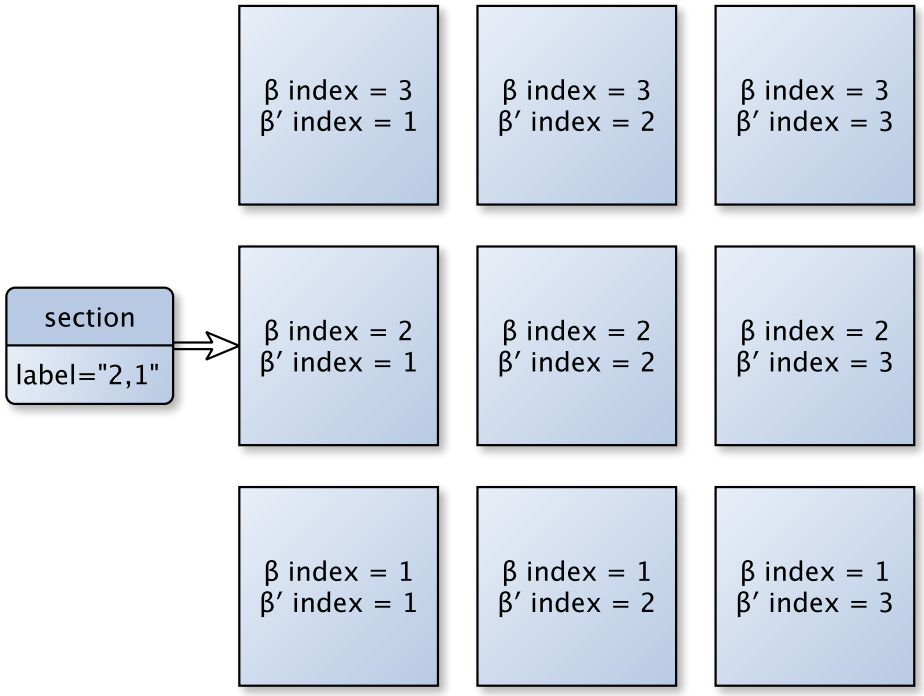
Format Proposal

- covarianceMatrix (one required): stores numerical values of covariance
- gridded2D (one required): already exists in the GND specification.



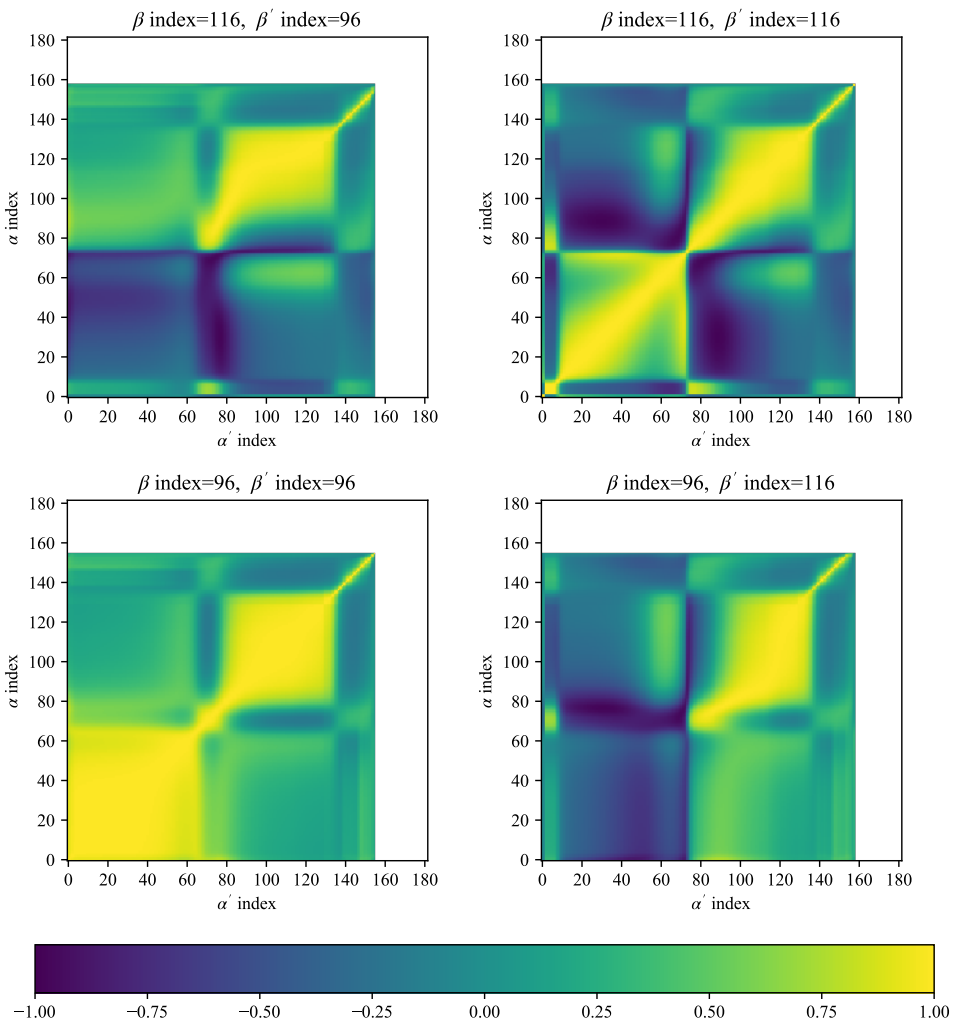
Format Proposal

- Once each section is defined, the full covariance matrix can be assembled under the covarianceSections node.
- In this example, there are three β values. Each pair of β and β' get a section. Each section is a covariance matrix between α and α'.



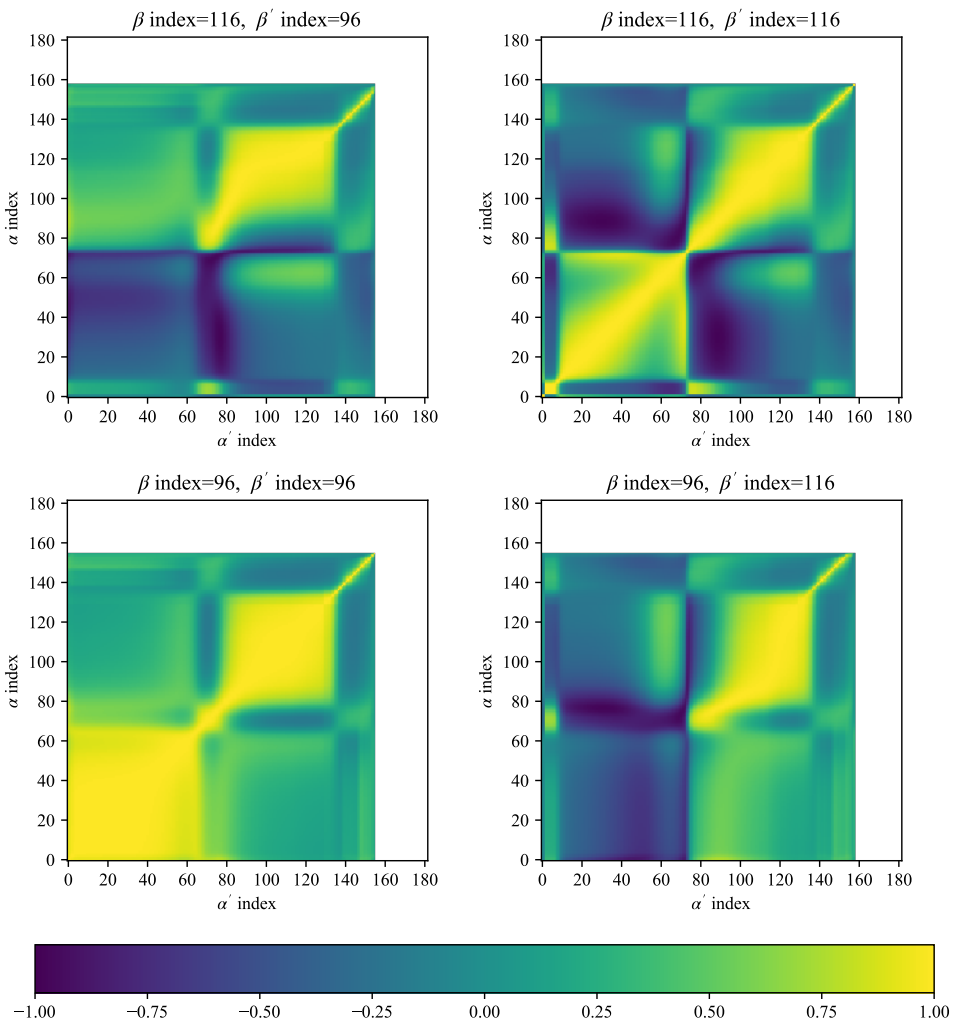
Demonstration

- 1000 random realizations of H in H2O were obtained from WPEC SG38 website.
- Same 182 α points and 259 β points from each realization.
- Covariance data was obtained using standard sample statistics.
- Full covariance matrix occupies about 17.78 GB in HDF5 format (double precision)
- Same data in XML will certainly be larger
- The proposed format allows for a coarser grid over covariance through rowData and columnData.



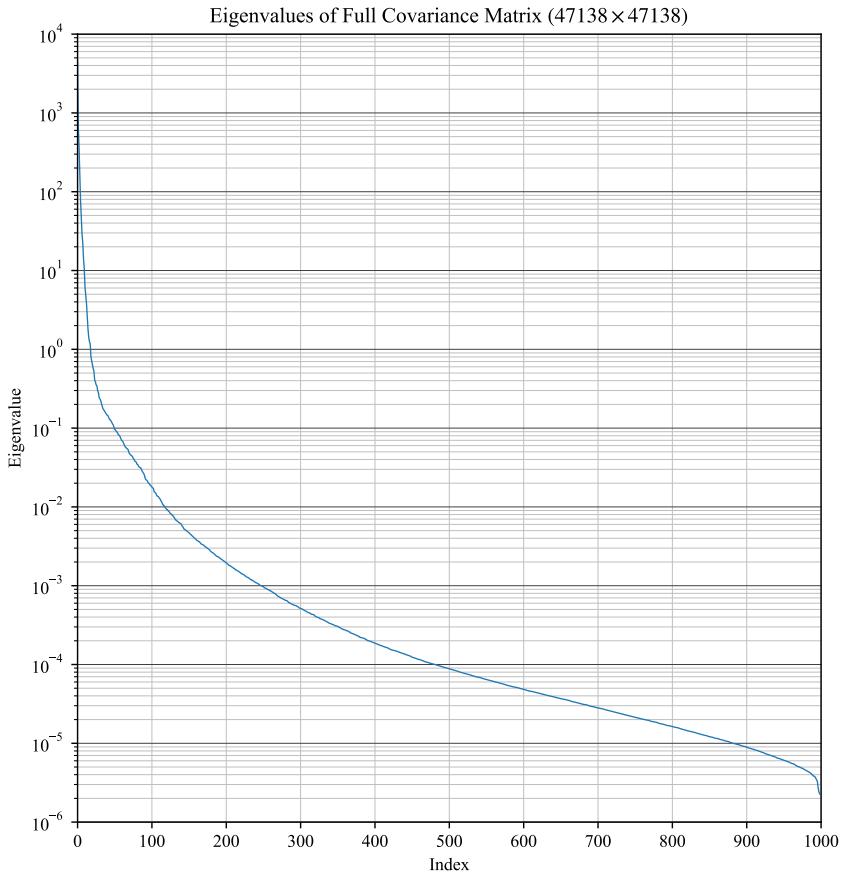
Demonstration

- The gridded2D container supports compression methods immediately applicable to covariance matrices.
- The symmetry attribute allows for storage of only $N(N+1)/2$ instead of N^2 entries.
- Values for α and β are over a fixed grid so some values of $S(\alpha, \beta)$ are undefined. A non-negligible number of covariances are therefore undefined. Undefined regions are whitespace in figure on the right.
- GND allows a submatrix to be embedded in an otherwise sparse matrix.



Future Work – Format

- The full covariance matrix can become prohibitively large.
- There may be ways to compress covariance data and store in GND format.
- A simple way would be to choose a coarser set of α and β values for the covariance matrix.
- Another way would be to perform PCA and store the first few components corresponding to the largest eigenvalues. The plot to the right shows the first 1000 eigenvalues of the full covariance matrix. The largest eigenvalue is 4.397E3. The magnitude of each eigenvalue falls below 1.0 after the the first 18 eigenvalues.



Future Work – Processing

- Implement ability to write GND files in SCALE.
- SCALE 6.3 has infrastructure in place for reading XML files in GND format:
  - QT for XML Parsing
  - C++ classes for low level containers and GND nodes
  - Data is written to AMPX in-memory data structures
- A format has been proposed for storing TSL data. Now we need to develop tools to encourage adoption of the format.