Recent Work on Thermal Scattering Covariance Generation and Compression

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Table of Contents

Motivation

- How does is a quantity f affected by uncertainty in $x_1, \ldots, x_N$?
- Expand f about $\tilde{f} = f(\tilde{x}_1, \ldots \tilde{x}_N)$:

$$f(x_1, \ldots, x_N) = \tilde{f} + \frac{\partial f}{\partial x_1}(x_1 - \tilde{x}_1) + \ldots + \frac{\partial f}{\partial x_N}(x_2 - \tilde{x}_N)$$

- Treating $x_1, \ldots, x_N$ as random variables, we have f as a weighted sum of random variables with variance

$$\mathrm{Var}(f) = \sum_i \left(\frac{\partial f}{\partial x_i}\right)^2 \mathrm{Var}(x_i) + \sum_{i \neq j} \frac{\partial f}{\partial x_i} \frac{\partial f}{\partial x_j} \mathrm{Cov}(x_i, x_j) \; .$$

- The partial derivatives $\partial f / \partial x_i$ are *sensitivities* and $\mathrm{Cov}(x_i, x_j)$ is the *covariance* between x_i and x_j.

Motivation

The Sandwich Formula

$$\mathrm{Var}\left(f\right) = \boldsymbol{s}^{\mathsf{T}} \boldsymbol{A} \boldsymbol{s}$$

where

$$\boldsymbol{s} = \begin{pmatrix} \frac{\partial f}{\partial x_1} \\ \vdots \\ \frac{\partial f}{\partial x} \end{pmatrix} \text{ and } \boldsymbol{A} = \begin{pmatrix} \mathrm{Cov}\left(x_1, x_1\right) & \cdots & \mathrm{Cov}\left(x_1, x_N\right) \\ \vdots & \ddots & \vdots \\ \mathrm{Cov}\left(x_N, x_1\right) & \cdots & \mathrm{Cov}\left(x_N, x_N\right) \end{pmatrix}$$

- End users compute $\boldsymbol{s}$.
- Evaluators provide covariances $\boldsymbol{A}$.
- The Evaluated Nuclear Data File format, ENDF-6 [1] provides file formats covariances for *some* types of nuclear data.

Thermal Scattering

Incoherent Inelastic Scattering

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

where

$$\alpha = \frac{E' + E - 2\mu\sqrt{EE'}}{Ak_B T} \text{ and } \beta = \frac{E' - E}{k_B T}.$$

- At energies (approximately less than $5\,\text{eV}$), thermal scattering takes place.
- The thermal scattering kernel $S\left(\alpha, \beta\right)$ is two dimensional data. The double differential scattering cross section $\sigma\left(E \to E', \mu\right)$ is actually three dimensional data.
- ENDF-6 does not currently specify a format for storing $S\left(\alpha, \beta\right)$ covariance.

Generalized Nuclear Data Format

- New data format [2] to eventually supersede ENDF-6
- Previous work developed a format in the Generalized Nuclear Data format for storing $S(\alpha, \beta)$ covariances.

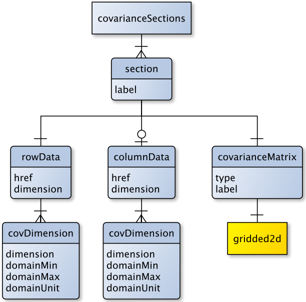


Figure: Structure of covariance data for thermal scattering data. From [3].

SCALE Implementation

- Implementation performed in AMPX [4] at GNDS Data Structures Level.
- Covariance for $S(\alpha, \beta)$ data is four dimensional.
- α and β indices are flattened to a linear index.
- Underlying data structure is a symmetric two dimensional matrix.

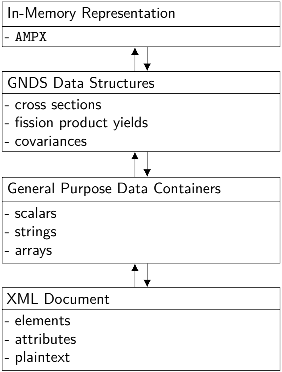


Figure: Hierarchy of abstraction layers for nuclear data in SCALE.

SCALE Implementation

- The base class `Covariance` is not necessarily symmetric to account for cross-covariance across different reactions.
- Existing classes updated to inherit from common base classes.

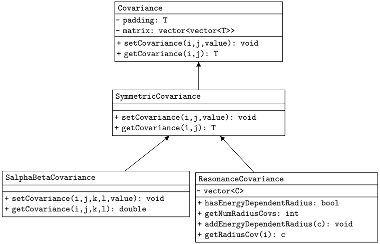


Figure: Covariance class inheritance

Generating $S(\alpha, \beta)$ Covariance Data

- Covariance data was generated from 1000 random realizations of H in H_2O.
- Full covariance matrix had $(182 \times 259)^2 \approx 2 \times 10^9$ entries.
- Full uncompressed covariance matrix occupied about 17.78 GB of storage as HDF5 file.
- GNDS format supports more than just α, β parameters. Adding one more dimension with just 10 points brings data storage into TB range.
- GNDS format supports basic compression methods. Sparsity and symmetric are immediately applicable.

	Min	Max	Points	Interpolation
α	0.0005	632.9	182	Lin-Log
β	0.0	158.1	259	Lin-Log

Table: Example TSL Data Dimensions

Principal Component Analysis

- Decompose the covariance matrix $\boldsymbol{A}$ into a unitary matrix of eigenvectors $\boldsymbol{U}$ and diagonal matrix of eigenvalues $\boldsymbol{\Lambda}$ by

$$\boldsymbol{A} = \boldsymbol{U}\boldsymbol{\Lambda}\boldsymbol{U}^\intercal \,.$$

- If $\boldsymbol{A}$ is of rank r, then there are r eigenvectors making up the columns of $\boldsymbol{U}$ and r eigenvalues making up the diagonal entries $\boldsymbol{\Lambda}$:

$$\boldsymbol{U} = \begin{pmatrix} | & & | & | & & | \\ \boldsymbol{u}_1 & \cdots & \boldsymbol{u}_r & \mathbf{0} & \cdots & \mathbf{0} \\ | & & | & | & & | \end{pmatrix} \quad \boldsymbol{\Lambda} = \mathrm{diag}\left(\lambda_1, \ldots, \lambda_r, 0, \ldots, 0\right)$$

- A low rank approximation of $\boldsymbol{A}$ can be created by keeping only $\tilde{r} < r$ eigenvalues in $\boldsymbol{\Lambda}$ and discarding the $r - \tilde{r}$ smallest eigenvalues.

Principal Component Analysis

- The amount of information lost is

$$\frac{\left\|\boldsymbol{A}-\tilde{\boldsymbol{A}}\right\|_2}{\|\boldsymbol{A}\|_2}=\frac{\sqrt{\sum_{i=\tilde{r}+1}^{r}\lambda_i}}{\sqrt{\sum_{i=1}^{r}\lambda_i}}=\sqrt{\frac{\sum_{i=\tilde{r}+1}^{r}\lambda_i}{\sum_{i=1}^{r}\lambda_i}}.$$

- Significant amount of information retained by keeping only a few eigenvalues

$\tilde{r}$	Information Lost	Memory Usage (MB)
0	100.00%	0.0
1	17.34%	0.3771
6	0.94%	2.263
121	0.000997%	45.63
1000	0.00%	377.1

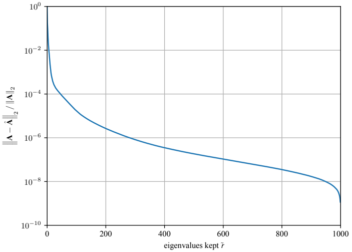
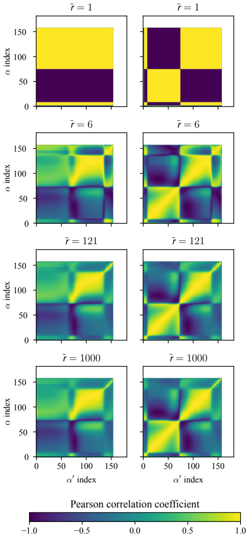


Figure: Frobenius norm of residual matrix $\boldsymbol{A}-\tilde{\boldsymbol{A}}$.

Principal Component Analysis

- Each sub-block has fixed β values and changing α values.
- The left column shows off-diagonal submatrices (corresponding to β indices $[116, 96]$).
- The right column shows on-diagonal submatrices (corresponding to β indices $[116, 116]$).
- Each row shows the approximated submatrix obtained by keeping the first $\tilde{r}$ largest eigenvalues.
- Values for which $S(\alpha, \beta)$ is undefined have no covariance



Conclusions

- Data structures for representing thermal scattering kernel covariances were implemented in AMPX.
- Covariance matrices will be quite large for practical problems.
- GNDS format already supports some methods of compression.
- Principal Component Analysis can take advantage of large singular values to further compress matrices.

Future Work

- Generate temperature dependent $S(\alpha, \beta, T)$ from perturbed probability density of states.
- Compute sensitivities for a benchmark problem.
- Propagate uncertainties in $S(\alpha, \beta, T)$ through benchmark problem.
- Quantify uncertainty due to uncertainty in $S(\alpha, \beta, T)$.

Acknowledgements

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