Update on Covariance Data Testing Strategy at LANL

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Towards an ENDF/B-VIII.0-based Covariance Library

**Processing** through NJOY’s ERRORR module

**Identifying** and **correcting** mathematical and physical deficiencies

**Communicating** across pipeline, from evaluator to end user

**Understanding** use cases and **interpreting** results

**Releasing** to customers
Motivation for Library

**Criticality Safety**
- Whisper code
- Safety limits

**Uncertainty Quantification**
- Sensitivity-based approaches ("sandwich rule")
- Sampling-based approaches (stringent requirements, distributions)

**Experiment Design**
- EUCLID project
- Validating data and detangling compensating errors
Challenges of Library Creation

Processing
• Covariance data has matured since NJOY development
• Code assessment and changes

Baseline
• No complete in-house past work
• No well-understood benchmarks
• Looking to outside work

Data Deficiencies
• Mathematical (negative eigenvalues, etc.)
• Physical (comparison to experimental unc., etc.)
• Incomplete data sets

Need to develop testing framework!
Approach to Testing

1. Interaction
2. Processing
3. Checks
   - Mathematical properties
   - Constraints
   - Physical bounds
4. Error propagation

Notes:

- This presentation is on strategy and building infrastructure, not results.
- Work first motivated by ENDF/B-VIII.0 but will be used for ENDF/B-VIII.1 betas.
- Looking for community feedback for collaboration.
Interaction

Needs

- Parse ENDF-formatted covariance data
- Build super-matrices from sub-matrices
- Identify what data is available in an evaluation
Interaction: ENDFtk

```python
import ENDFtk

tape = ENDFtk.tree.Tape.from_file('n-094_Pu_239.endf')
section = tape.MAT(9437).MF(33).MT(18).parse()

# I know there's only one SquareMatrix subsubsection
matrix = section.reactions[0].explicit_covariances[0]
print(matrix.energies, matrix.values)
```
Processing

NJOY/ERRORR

• Robust and powerful but predates modern covariances

• Errors: evaluation or NJOY?
  − Examples: Fe-54, O-16

• QA checks
  − Consistency between relative and absolute
  − Running on evaluation grid
  − Processed values between evaluation values
Checks: Mathematical Properties

Requirements
• Positive definite
• Symmetric
• Correlations in [-1, 1]

Gray Areas
• Large relative uncertainties
• Implied asymmetric distributions
• Roundoff issues

\[
corr(X) = \begin{bmatrix}
1 & \frac{E[(X_1 - \mu_1)(X_2 - \mu_2)]}{\sigma(X_1)\sigma(X_2)} & \cdots & \frac{E[(X_1 - \mu_1)(X_n - \mu_n)]}{\sigma(X_1)\sigma(X_n)} \\
\frac{E[(X_2 - \mu_2)(X_1 - \mu_1)]}{\sigma(X_2)\sigma(X_1)} & 1 & \cdots & \frac{E[(X_2 - \mu_2)(X_n - \mu_n)]}{\sigma(X_2)\sigma(X_n)} \\
\vdots & \vdots & \ddots & \vdots \\
\frac{E[(X_n - \mu_n)(X_1 - \mu_1)]}{\sigma(X_n)\sigma(X_1)} & \frac{E[(X_n - \mu_n)(X_2 - \mu_2)]}{\sigma(X_n)\sigma(X_2)} & \cdots & 1
\end{bmatrix}
\]
Checks: Constraints

Summation

- Normalized quantities stay normalized (e.g., PFNS)
- Total is sum of partials
  - NI-type
  - Overspecification
  - Missing channels

Tough Questions:

- What can be fixed during library generation?
- What requires rejecting an evaluation?

\[ \hat{F}_{k,k'} = F_{k,k'} - S_k Y'_{k'} - S_{k'} Y_k + Y_k Y'_{k'} \sum_j S_j. \]
Checks: Physical bounds

Sources

• Expert judgment limits set by D. Smith in: “Guidance on Generating Neutron Reaction Data Covariances for the ENDF/B Library”
• Lower limits defined by Neutron Data Standards uncertainties if a reaction is pre-dominantly measured relative to a specific standard
• Limits defined by templates of expected measurement uncertainties
• Spread in differential data
• Physical Uncertainty Boundary method limits (Neudecker, EPJ N 6, 19 2021).

Useful warnings or “hard stop” errors?
Checks: Physical bounds

- **Sanity check # 1:**
  Don Smith defined lower limits based on expert judgment given his experimental background.

- **Sanity check # 2:**
  Compare to standards’ unc. (e.g., most $^{239}$Pu nu-bar data measured relative to $^{252}$Cf)
Sanity check #3: Templates of expected measurement unc.

Sanity check #4: Compare against spread of experimental data (critical barrier: no easy access to curated data)

Sanity check #5: Physical Uncertainty Boundary method (work in progress)
Error Propagation

“Sandwich Norms”
• Simple problems for A/B comparisons
• Assess if processing-based changes have large impact

Benchmarks
• Propagate uncertainties to ICSBEP benchmarks, etc.
• Previous work by ORNL
• Goal: impact of new evaluations, consistency of independent efforts
• Important: unadjusted covariances
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Summary

Motivations

• Processed library for user applications
  – Sandwich rule and sampling
  – Continuous and MG
  – Fast and thermal
• Test ENDF/B-VIII.1 betas as they are released

Testing Approach

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2. Processing
3. Checks
   – Mathematical properties
   – Constraints
   – Physical bounds
4. Error propagation