Los Alamos NATIONAL LABORATORY

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

Experiment Design

- EUCLID project
- Validating data and detangling compensating errors

Uncertainty Quantification

- Sensitivity-based approaches (“sandwich rule”)
- Sampling-based approaches (stringent requirements, distributions)

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

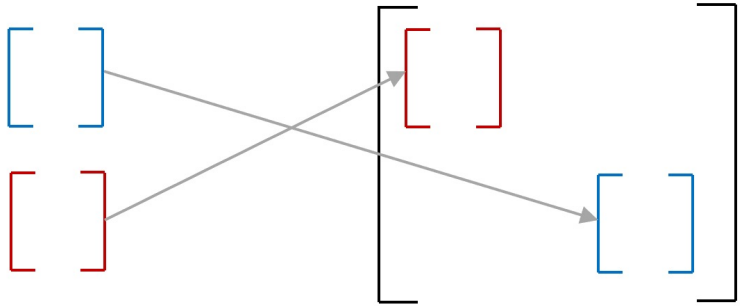
Notes:

- 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)
```


```
                                                                   9437 0  0
9.423900+4 2.369986+2          0          0          0          1943733  1
0.000000+0 0.000000+0          0          1          0          1943733  1
0.000000+0 0.000000+0          1          5       1953         62943733  1
1.000000-5 2.500000+3 1.000000+4 3.000000+4 5.000000+4 1.000000+5943733  1
1.500000+5 2.000000+5 2.500000+5 3.000000+5 3.500000+5 4.000000+5943733  1
4.500000+5 5.000000+5 5.500000+5 6.000000+5 6.500000+5 7.000000+5943733  1
7.500000+5 8.000000+5 8.500000+5 9.000000+5 1.000000+6 1.200000+6943733  1
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4.500000+6 5.000000+6 5.500000+6 6.000000+6 6.500000+6 7.000000+6943733  1
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1.050000+7 1.100000+7 1.150000+7 1.200000+7 1.250000+7 1.300000+7943733  1
1.350000+7 1.400000+7 1.450000+7 1.500000+7 1.550000+7 1.600000+7943733  1
1.650000+7 1.700000+7 1.750000+7 1.800000+7 1.850000+7 1.900000+7943733  1
1.950000+7 2.000000+7 0.000000+0 0.000000+0 0.000000+0 0.000000+0943733  1
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0.000000+0 0.000000+0 0.000000+0 1.432642-3 8.050435-4 7.035717-4943733  1
6.920263-4 6.910049-4 6.922385-4 6.910509-4 6.901216-4 6.885557-4943733  1
6.858096-4 6.811286-4 6.734839-4 6.636951-4 6.500609-4 6.335326-4943733  1
6.147588-4 5.948409-4 5.748259-4 5.557599-4 5.384533-4 5.233560-4943733  1
5.020184-4 4.920090-4 5.266489-4 5.686596-4 5.444514-4 5.162471-4943733  1
5.056617-4 5.009940-4 4.902230-4 4.752272-4 4.650518-4 4.635846-4943733  1
4.685851-4 4.758673-4 4.816964-4 4.850962-4 4.810040-4 4.781452-4943733  1
4.783864-4 4.822776-4 4.894792-4 4.992777-4 5.108826-4 5.235039-4943733  1
5.362219-4 5.479424-4 5.574949-4 5.639292-4 5.667455-4 5.661101-4943733  1
5.627336-4 5.575615-4 5.515868-4 5.455555-4 5.399483-4 5.349451-4943733  1
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4.586614-4 4.551866-4 4.507886-4 4.443359-4 4.363390-4 4.270795-4943733  1
4.171739-4 4.071737-4 3.976781-4 3.891105-4 3.817094-4 3.716475-4943733  1
3.682984-4 3.863655-4 4.036600-4 3.887004-4 3.731767-4 3.667487-4943733  1
3.630719-4 3.550991-4 3.435137-4 3.339874-4 3.294224-4 3.287005-4943733  1
3.295369-4 3.304832-4 3.316757-4 3.278339-4 3.272876-4 3.309279-4943733  1
3.384984-4 3.491569-4 3.619405-4 3.759954-4 3.905825-4 4.049153-4943733  1
```
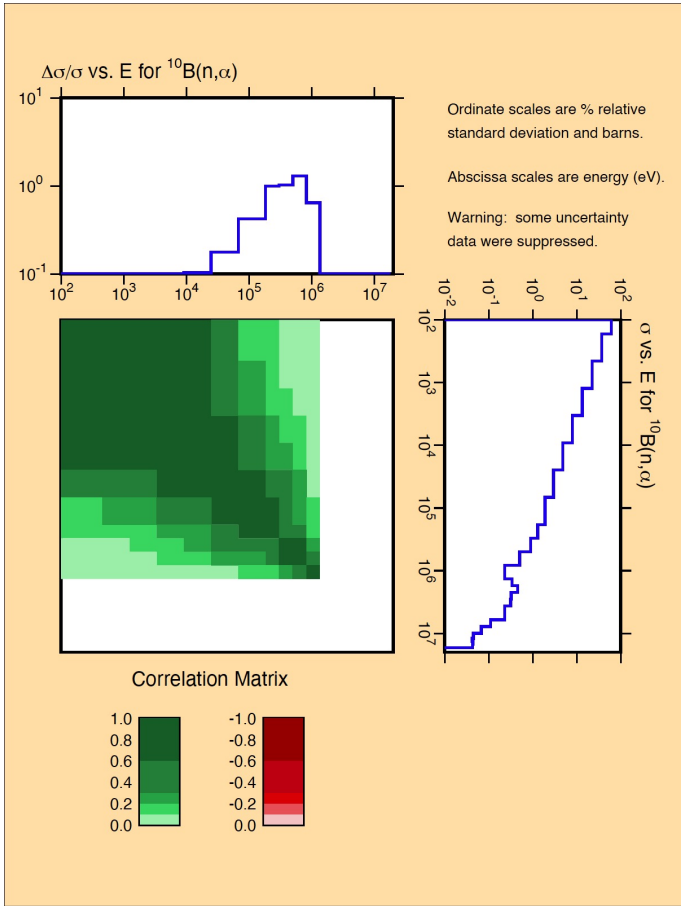

Processing

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

$$\operatorname{corr}(\mathbf{X}) = \begin{bmatrix} 1 & \frac{\mathrm{E}[(X_1-\mu_1)(X_2-\mu_2)]}{\sigma(X_1)\sigma(X_2)} & \cdots & \frac{\mathrm{E}[(X_1-\mu_1)(X_n-\mu_n)]}{\sigma(X_1)\sigma(X_n)} \\ \frac{\mathrm{E}[(X_2-\mu_2)(X_1-\mu_1)]}{\sigma(X_2)\sigma(X_1)} & 1 & \cdots & \frac{\mathrm{E}[(X_2-\mu_2)(X_n-\mu_n)]}{\sigma(X_2)\sigma(X_n)} \\ \vdots & \vdots & \ddots & \vdots \\ \frac{\mathrm{E}[(X_n-\mu_n)(X_1-\mu_1)]}{\sigma(X_n)\sigma(X_1)} & \frac{\mathrm{E}[(X_n-\mu_n)(X_2-\mu_2)]}{\sigma(X_n)\sigma(X_2)} & \cdots & 1 \end{bmatrix}.$$

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?

$$\widehat{F}_{k,k'} = F_{k,k'} - S_k Y_{k'} - S_{k'} Y_k + Y_k Y_{k'} \sum_j S_j .$$

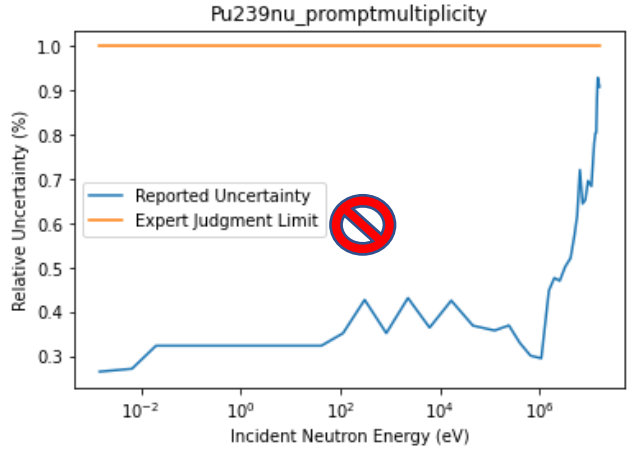
Checks: Physical bounds

Sources

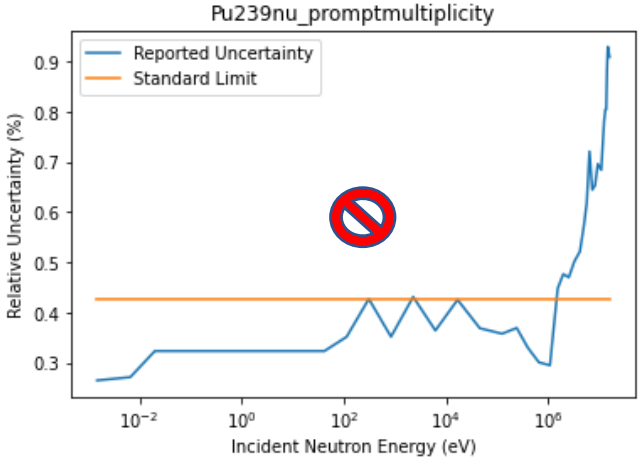
- Expert judgment limits set by D. Smith in: “Guidance on Generating Neutron Reaction Data Covariances for the ENDF/B Library”
- Lower limits defined by Neutron Data Standards uncertainties if a reaction is pre-dominantly measured relative to a specific standard
- Limits defined by templates of expected 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

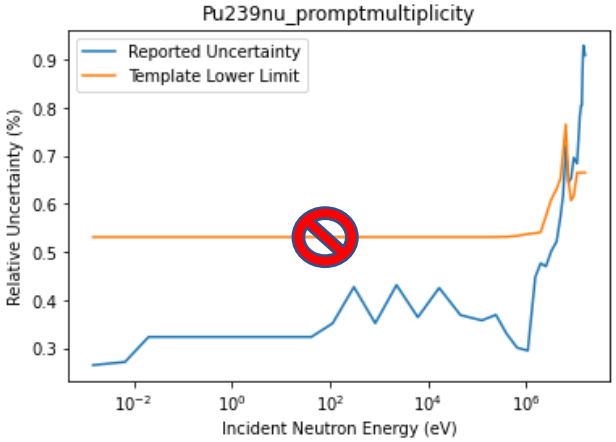


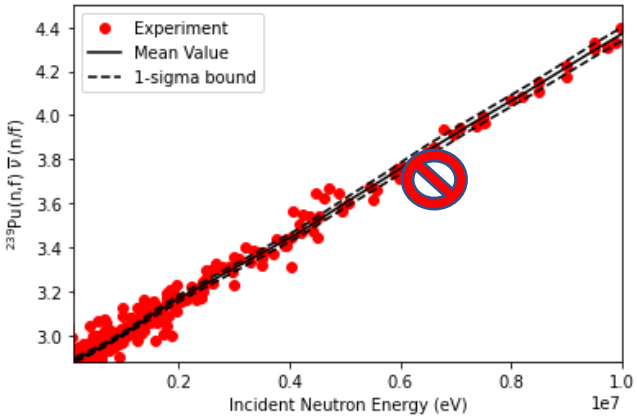
- Sanity check # 1:
  Don Smith defined lower limits based on expert judgment given his experimental background.

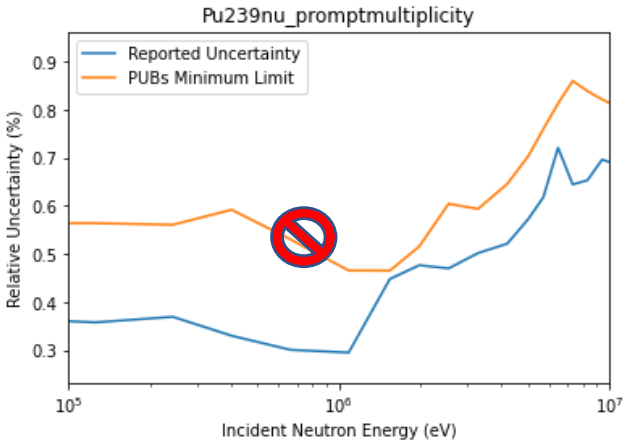


- Sanity check # 2:
  Compare to standards' unc. (e.g., most ^{239}Pu nu-bar data measured relative to ^{252}Cf)

Checks: Physical bounds







<u>Sanity check #3:</u>
Templates of expected measurement unc.

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

<u>Sanity check #5:</u>
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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Funding Sources

- Advanced Simulation and Computing Program
- Nuclear Criticality Safety Program

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

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