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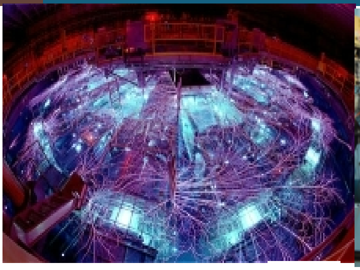
Sandia National Laboratories

User Challenges with Covariance Data



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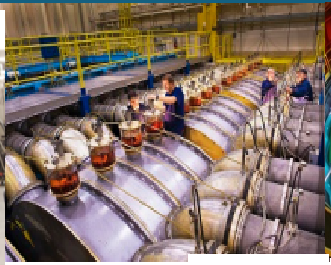

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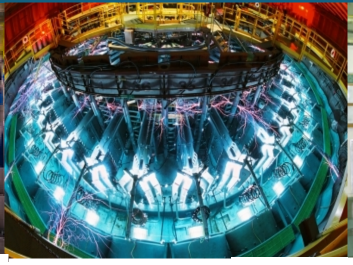

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ACRR

PRESENTED BY

Patrick Griffin, Laboratory Fellow, Org. 1000

Oct. 11, 2022

Nuclear Data Uncertainty Quantification Meeting (NDUQWM) October 11-13, 2022

R&A#: xxxx

Approved for Unlimited Release

Name/Org: Patrick Griffin/SNL Date: 09/30/2022
Guidance (if applicable) ________________

U.S. DEPARTMENT OF ENERGY NNSA

Agenda

- Identify the Nuclear Data Contacts at Sandia
- Highlight Sandia Mission Areas that Use Nuclear Data
- My view of the highest covariance challenges the user community faces

The SNL NDWG webpage has more details and points to publications.

Sandia's NDWG Representatives

- Radiation Effects: Patrick Griffin, Lab Fellow, Advanced Science and Technology Division, Org. 1000

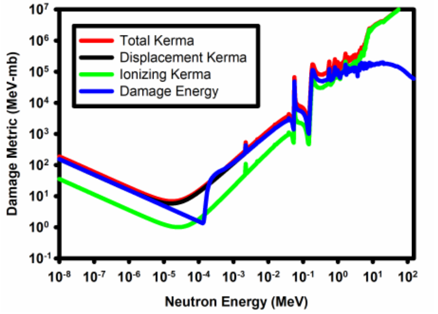
- Nuclear Forensics: Philip Dreike, Senior Scientist, Space Ground Systems Program, Org. 6740

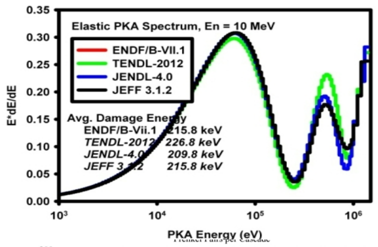
- SNL NDWG Website: https://sandia.gov/nuclear-data/home-snl-ndwg

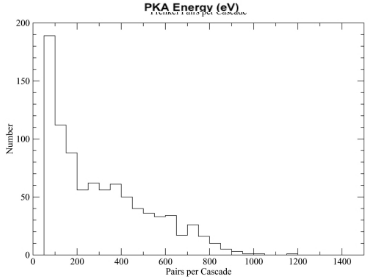
- Ph.D. in nuclear physics from Ohio University in 1979.
- Over 40 years experience: in radiation modeling, neutron effects testing, radiation dosimetry, and radiation damage to materials.
- ASTM Fellow (Award of Merit)
- Appointment as National Associate of the National Academies
- U.S. representative for several IAEA-sponsored CRPs.
- Sandia Editor for the Defense Research Review. (DRR)

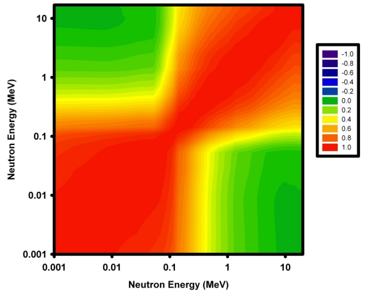
Key Sandia Nuclear Data Needs for Important Missions

- Radiation damage to semiconductors:
  - Main semiconductor materials: Si, GaAs, GaN, SiGe, SiC
  - Other materials:
    - Semiconductors: [$HfSe_2$]; Dielectrics: [SIO_2, HfO_2, $Hd_{0.5}Zr_{0.5}O_2$]; Dopants: [B, P, Sb, In]; Metals: [Au, Cu, W]; Capacitors [Ta, gel];
- Radiation damage metrics:
  - Displacement kerma; Frenkel pair production; defect evolution
  - Stochastics of radiation damage
  - Trapped charge; charge recombination
  - Recoil spectra
  - LET distributions
- Uncertainties in damage metrics:
  - Cross reaction correlations
- Relationship between a calc. damage metric and an observed damage mode









There are many nuclear data aspects to consider, e.g., how the data is used.

Covariance Challenges Users Face:

- My ENDF-extracted correlation matrix is not positive semi-definite!
- I need to rebin the covariance matrix into a different energy group structure.
- Treatment of angular dependent correlations with only the P1 term may not be adequate.
- I have large uncertainties and get unphysical values when I sample, i.e., negative cross sections or cosine values > 1.
- I have an input quantity that is, based on the physics considerations, not normally distributed. How do I propagate the resulting uncertainties?
- The covariances I get seem to be too small to represent the quantity.
- How do I address uncertainty in the recoil spectra. ENDF-6 does not even support covariance matrices for recoil spectra.
- So, I have to use a TMC approach, but I do not have random libraries for the nuclides of interest.
- How do I obtain the cross-isotope correlation data?
- How do I generate prior (calculated) neutron spectra covariances so that I can propagate uncertainty in response metrics?
- How do I generate covariance matrices for stopping power, damage partition function, etc.?

We face a wide range of challenges – many that can be addressed with improved processing codes and support tools.

Discussion of Issue 1:

- **Issue: My ENDF-extracted correlation matrix is not positive semi-definite!**

- **Considerations:**
  - A common occurrence – at Sandia and elsewhere.
    - Seen in fine group representations (>400 groups) even when using double precision.
  - Often results from precision limitations in data representation or in rebinning processes.
  - Easily addressed/fixed – via a Cholesky transformation

- **Related Issues:**
  - For spectra, there is also a unity normalization constraint. This imposes a summation constraint on the rows of a correlation matrix.
  - Here, the ENDF-6 Manual tells us what to check this normalization constraint and how to fix this if required.
  - Add this explicit guidance to the ENDF-6 Manual for the MF6 correlation data – and improve accuracy of code processing and results reporting.

Solution: algorithm improvements in processing codes and ENDF-6 Manual guidance.

Discussion of Issue 2:

- **Issue: I need to rebin the covariance matrix into a different energy group structure.**

- **Considerations:**
  - This two-dimensional interpolation can be a challenge.
  - This is a common need, but the current version of codes such as NJOY-2016 (ERRORR/COVR modules) support this need.
  - The real issue may be problems with the resulting positive semidefinite attribute for the rebinned matrix. I see this all the time for dosimetry covariances and fission neutron spectra processed using NJOY-2016. This was addressed in Issue 1.

- **Related Issues:**
  - See Issue 1.

Solution: Improvements in NJOY-2016 processing code. More visibility about NJOY-2016 capabilities.

Discussion of Issue 3:

- **Issue: Treatment of angular dependent correlations with only the P1 term may not be adequate.**

- **Considerations:**
  - An important issue discussed at the recent CW2022 workshop.
  - NJOY – and MF34 – express this covariance only through the P1 component.
  - ENDF-6 Manual states:
    - "It is judged that covariances between the magnitude and shape are likely to be important only when theory plays a strong role in an evaluation." A condition that is more often true tese days.
    - "the covariance matrix in File 34 may refer to Legendre coefficients in the LAB coordinate system even when the data in File 34 are given in the CM coordinate system."
    - "In ENDF-6 formats there is no provision for covariance components linking the angular distribution parameters for different materials, … but is normally zero." Given modern codes, is this still true?

- **Needs:**
  - Verify sufficiency of current approximations – requires some treatments that address the actual angular distribution – probably through TMC.

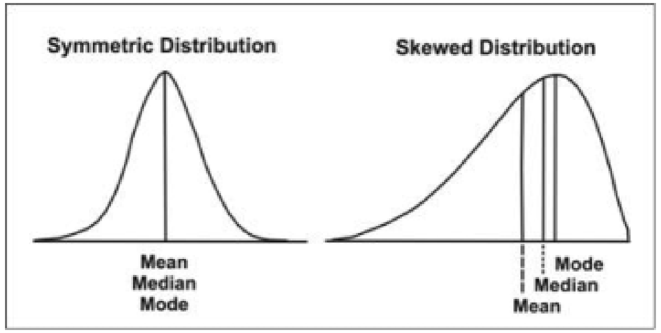
Path Forward: ENDF-6 format extensions.

Discussion of Issue 4:

- **Issue: I have large uncertainties and get unphysical values when I sample, i.e., negative cross sections or cosine values >+1 or <-1.**

- **Considerations:**
  - Yes, the assumption of a normal distribution breaks down when there are parameter range constraints.
  - Normal/Gaussian distributions are typically used because they have easy analytic forms to support uncertainty propagation.
    - [Median = Mode = Average] for Normal distribution
  - Alternate distributions include truncated Gaussian, log-normal, Gamma distribution, etc.
  - When uncertainties are large, use of a log-normal distribution produces a bias – relative to use of a normal distribution.

Solution: Use the most physically meaningful distribution for your application. If not Gaussian, take the effort to properly propagate the uncertainty.



Discussion of Issue 5:

- **Issue: I have an input quantity that is, based on the physics considerations, not normally distributed. How do I propagate the resulting uncertainties?**

Type of $pdf_{\xi'}$	Transformation: $q(\xi) =$
Normal(μ, σ)	$\mu + \sigma\xi$
Uniform(a, b)	$a + (b-a)\left(\frac{1}{2} + \frac{1}{2}\text{erf}(\xi\sqrt{2})\right)$
Log-normal(μ, σ)	$\exp(\mu + \sigma\xi)$
Gamma(a, b)	$ab\left(\xi\sqrt{\frac{1}{9a}} + 1 - \frac{1}{9a}\right)^3$
Exponential(λ)	$-\frac{1}{\lambda}\log\left(\frac{1}{2} + \frac{1}{2}\text{erf}\left(\frac{\xi}{\sqrt{2}}\right)\right)$

- **Considerations:**
  - With great difficulty!
  - Even with normal distributions, uncertainty propagation can be challenging when nonlinear expressions are involved.
    - Linear function of normal distributions have an exact uncertainty propagation
    - Complex expressions are approximated using a Taylor series expansion
  - Alternate formulations exist for log-normal. Others can be derived for specific distributions.
    - Transformations can turn Gaussian distributions into many other distributions.
  - If the distribution is general (not analytical), you probably need to do TMC with random sampling.

Solution: Better tools for handling non-Normal distributions need to be made more generally available.

Discussion of Issue 6:

- **Issue: The covariances I get seem to be too small to represent the quantity/parameter.**

- **Considerations:**
  - A common problem.
  - Probably reflects model defect (in models) or unrecognized sources of uncertainty (USU) (in experiments).
  - Look harder at the sources of uncertainty. Add SME-based uncertainty components to address unrecognized uncertainty contributions.
  - Consult with others to confirm the conflict and to help isolate the deficiencies in the uncertainty characterization.

Path Forward: Socialize the issue.

Discussion of Issue 7:

- **Issue: How do I address uncertainty in the recoil atom spectra. ENDF-6 does not even support covariance matrices for recoil spectra.**

- **Considerations:**
  - A significant issue for Sandia response analysis.
  - Interim approaches:
    - Estimate uncertainty through library comparison.
    - Address using TENDL random libraries and TMC – but variation seems too small (see Issue 6).

- **Implications:**
  - Cost/benefit of addressing ENDF-6 format restrictions are marginal. Look forward and address within the context of GNDS format.
  - Need more experimental data to validate models.

Path Forward: Look to emerging GNDS format. Incorporate data for some trial isotopes and encourage community to develop processing tools.

Discussion of Issue 8:

- **Issue: So, I have to use a TMC approach, but I do not have random libraries for the nuclides of interest.**

- **Considerations:**
  - At Sandia, we have approached Dimitri Rochman and Arjan Koning to provide needed files for Silicon.
  - At Sandia, we should gain competence in using TALYS and the T6 Software System [TEFAL, TASMAN] so we can generate our own random files.

- **Complications:**
  - What do I do for the low-Z isotopes where, for low threshold energy reactions, the calculations cannot be trusted, e.g., N important for GaN response metrics?

Path Forward: Support the Nuclear Data Pipeline. Develop more in-house ND expertise.

Discussion of Issue 9:

- **Issue: How do I obtain cross-isotope correlation data?**

- **Considerations:**
  - This has been done for special cases by Dimitri Rochman – and published, e.g., for silicon and tin.
  - The priority for this needs to be established.
    - What range of applications require consideration of cross-isotope correlations?
    - Since the cross-isotope correlation is probably only of concern for close A/Z nuclides, does this only need to be considered for elemental damage response modes?

- **Complication:**
  - What about materials, like GaAs, where the two critical elements are very close in A/Z?

Path Forward: Establish priority – then plan tool development/maturation.

Discussion of Issue 10:

- **Issue: How do I generate *a priori* (calculated) neutron spectra covariances so that I can propagate uncertainty in response metrics?**

- **Considerations:**
  - Uncertainties are assigned using subject-matter expertise (SME) and past experience.
  - Correlation matrices follow the published process of functional fits, e.g., see by Williams or Trkov published work.
    - Fit to basis functions, e.g., Maxwellian, $1/E^{[1-a]}$, Madland-Nix fission, Gaussian fusion. Fit parameter uncertainty to match SME standard deviations. Use MC methods to sample parameter space, normalize to unity, form MC-based correlation matrix. Apply to calculated spectrum.

- **Related Issues:**
  - Published efforts to use radiation transport tools, e.g., MCNP, have failed miserably to produce credible energy-dependent uncertainties. See Issue 6.
    - Deficiencies in modeling uncertainty for spatial dimensions and material impurities may have been an issue.
    - The new versions of MCNP are expected to implement new options that support this application.

Path Forward: Validate approach for a wider range of neutron spectra. Look to future radiation transport sensitivity studies to support establishing a quantitative basis for energy-dependent standard deviations.

Discussion of Issue 11:

- **Issue: How do I generate covariance matrices for stopping power, damage partition function, etc.?**

- **Considerations:**
  - A Total Monte Carlo (TMC) approach is probably required.
  - Examples for silicon metrics (kerma, displacement, LET distributions) have been published.
  - Aspects of parameter correlation were shown to be critical – over 2X change.

- **Related Issues:**
  - Sources of uncertainty in stopping power are a challenge.
    - Experimental data not available for many ion/target combinations of interest.
    - Model uncertainty, e.g., for DPASS or CasP, codes is an area that should be addressed.
  - Correlations between stopping power for different materials needs to be addressed.
  - Cascades in polyatomic lattices with dissimilar A/Z components needs to be refined.

Path Forward: This area is accessible with current tools. It just needs attention/priority.

Questions?