Mubar Covariances

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Outline

- What is “mubar” (the average of μ) , anyway?
- Which MF 34 Mubar covariances in ENDF/B VIII.0 have we studied?
- Problems with the O-16 mubar covariances
- Problems with Sensitivities between MCNP and SENSMG
- Uncertainty Results with O-16 and Pu-239
- Future Work

What is “mubar” anyway?

- For this paper, we are focusing on multi-group applications
- In terms of the cosine ($-1 \leq$ mubar ≤ 1), it is the average lab frame scattering angle for the neutron in elastic scattering
- When mubar is positive, the lab scattering is more forward, the mfp is longer, and the overall neutron leakage is increased
- When mubar is negative, the lab scattering is more backward, the mfp is shorter, and the overall neutron leakage is decreased
- Unlike cross section uncertainties and sensitivities, mubar does NOT directly affect the reaction rates
  - Mubars interact with the P1 fluxes → leakage rates
  - Cross sections interact with the P0 fluxes → reaction rates

Definition of mubar

- As given in the evaluation files and then processed in NJOY, mubar is given by incoming group – and its value includes the sum of all outgoing group cross sections.
- For a specific incoming group:
  - Mubar = (sum of outgoing P1 elastic xs) / (sum of outgoing P0 elastic xs)
  - Includes up-scatter (if present), self-scatter, and down-scatter
- NJOY only calculates the P1 contribution for mubar.

- Therefore, for each incoming group (for elastic scattering):
  - We have a given mubar (mean, or the average)
  - We have an uncertainty for mubar for each incoming group (variance or standard deviation – diagonal elements of the covariance matrix)
  - We have cross terms for different groups within the isotope (the off-diagonal elements of the covariance matrix)
  - No cross terms across isotopes – only 1 isotope at a time

Mubar covariances (mf 34) studied so far:

- Pu-239 from ENDF/B VIII
  - Processes through NJOY just fine
- U-235 from ENDF/B VIII
  - NJOY can't handle the formats used in the evaluation file
  - *a "to do" task has been noted for NJOY development*
- O-16 from ENDF/B VIII
  - Processes through NJOY just fine
  - BUT, the uncertainties are way too large – much larger than the -1 to +1 range at low energy and at certain resonance energies
  - Problem (probably) first reported at CSEWG 2018 by Pino Palmiotti
- O-16 from JENDL 4.0
  - Processes through NJOY just fine

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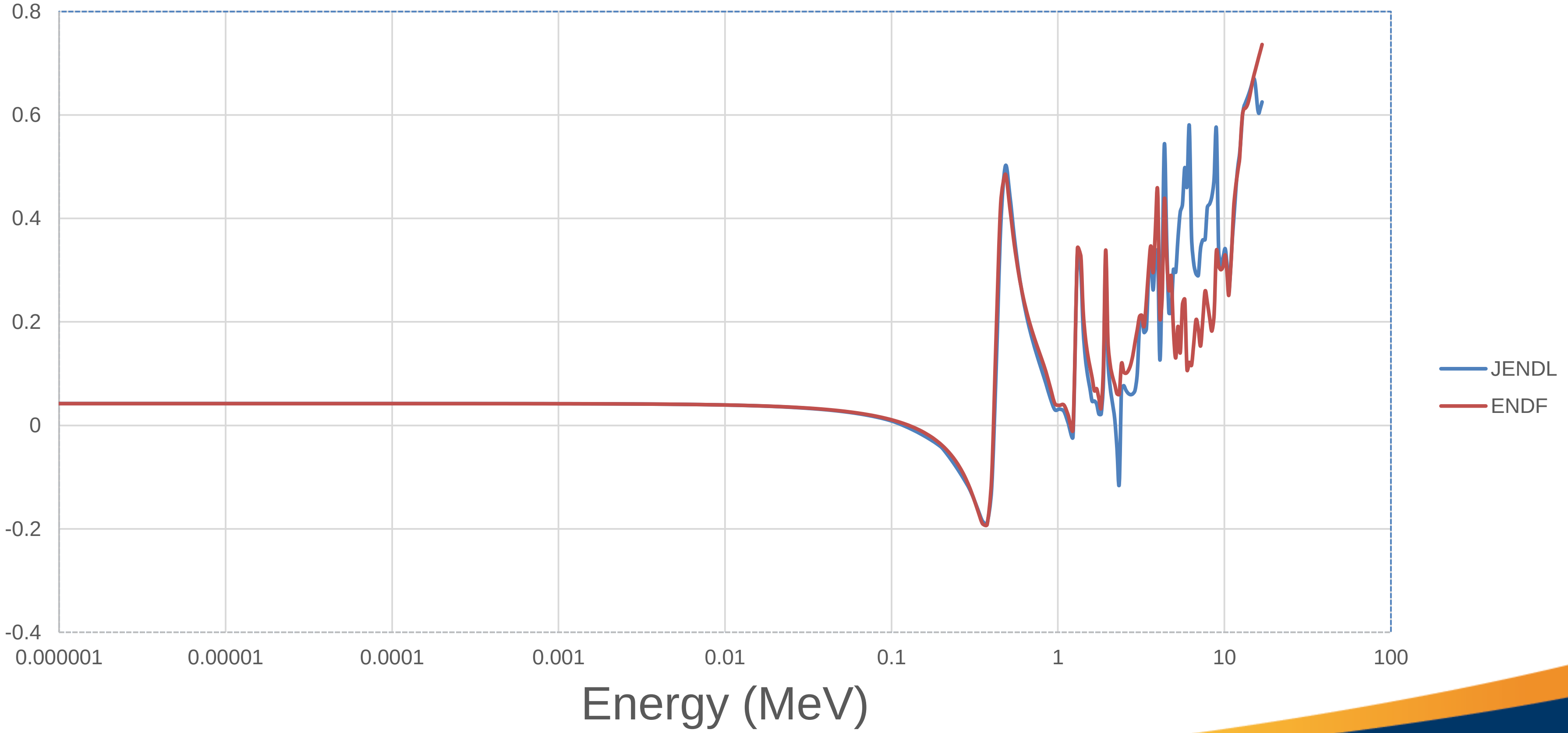
Problems with O-16 mubar variances

- ENDF/B VIII O-16 mubar covariance data stops at 7 MeV
  - It is because more reaction channels open up for O-16 at these high energies
    - Complicates R-matrix theory
  - The Japanese O-16 mubar covariance data goes at least to 17 MeV
- ENDF/B VIII O-16 mubar covariance data has very large uncertainties at lower energies* and at selected high energy resonance points
  - The Japanese O-16 mubar covariance data is 0.0 below 2.53e-8 MeV and small at energies just above room temperature

- BTW, for μ, (not the covariance of μ), ENDF/B VIII and JENDL 4.0 are reasonably consistent

- * *(this has been recently fixed at Los Alamos by Gerry Hale)*

O-16 elastic scattering mubar



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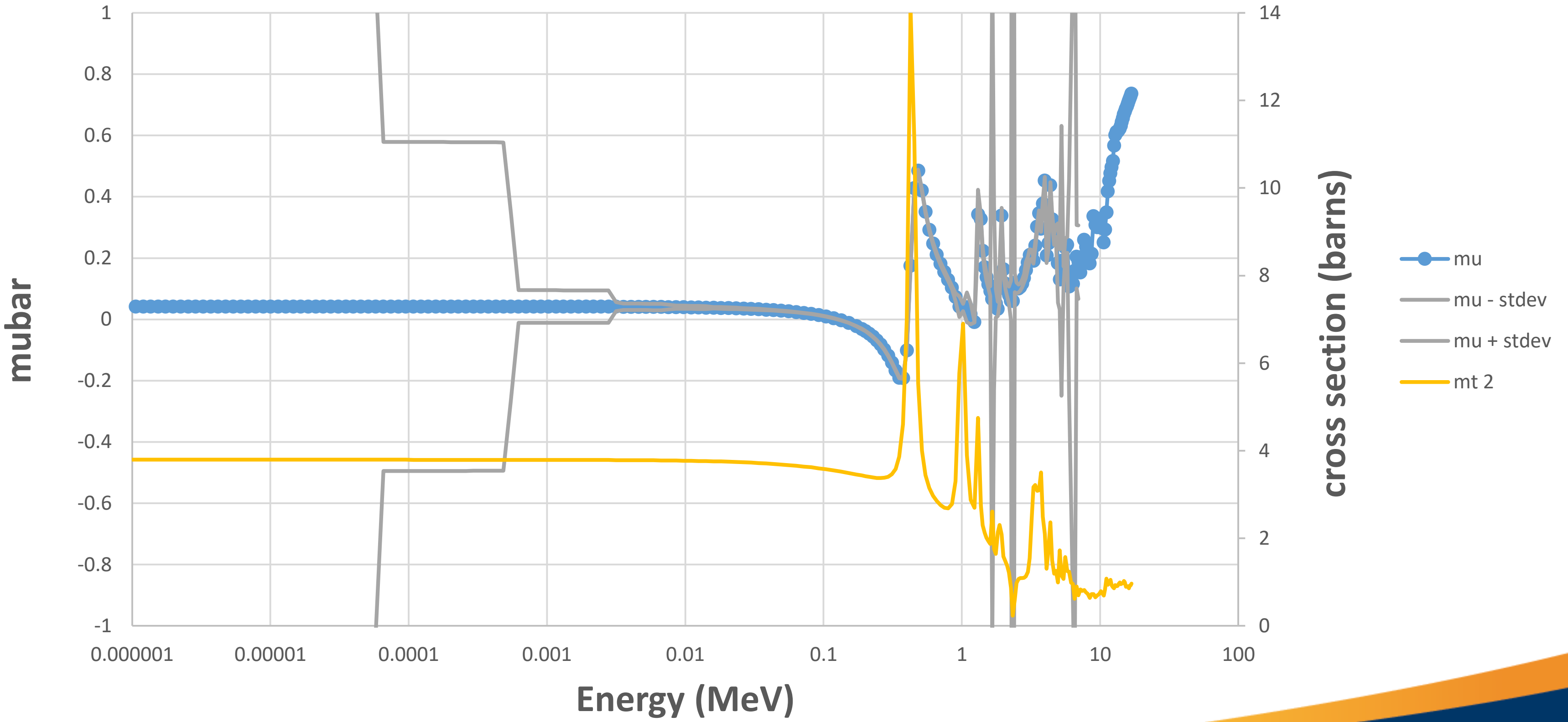
ENDF/B VIII.0
O16 XS, mubar and +/- 1 stdev



Sensitivity Vectors for the Sandwich Rule

- Sensitivities (e.g., % delta k / % delta x) are (1) a first order derivative and (2) problem dependent

- In MCNP Continuous Energy Monte Carlo
  - For k_{eff} problems, use the "ksen" option
  - For fixed source problems, use the "pert" option
  - All individual cross sections may be accessed for sensitivities (*but what about the P0, P1, P2… Legendre moments?*)
  - Accumulate the multi-group sensitivities with multi-group bin boundaries in the tallies
- In Multi-group Sn
  - Use Jeff Favorite's "SENSMG" code (which uses Partisn forward and adjoint calculations)
  - Some cross section are **not** available (*yet*)
    - Elastic, Inelastic, (n,2n), (n,3n), … are already mixed together in the Legendre scattering matrices used in Sn
    - Sensitivities with respect to P0, P1, P2, and P3 "scattering" moments are available
- Lot of experience shows that these 2 methods produce similar results – they both use adjoint fluxes in combination with forward fluxes.

- *In both Monte Carlo and Sn, sensitivities can also be estimated by 2 forward calculations (high and low) and then using a 2nd order accurate central difference estimate of the first order derivative*

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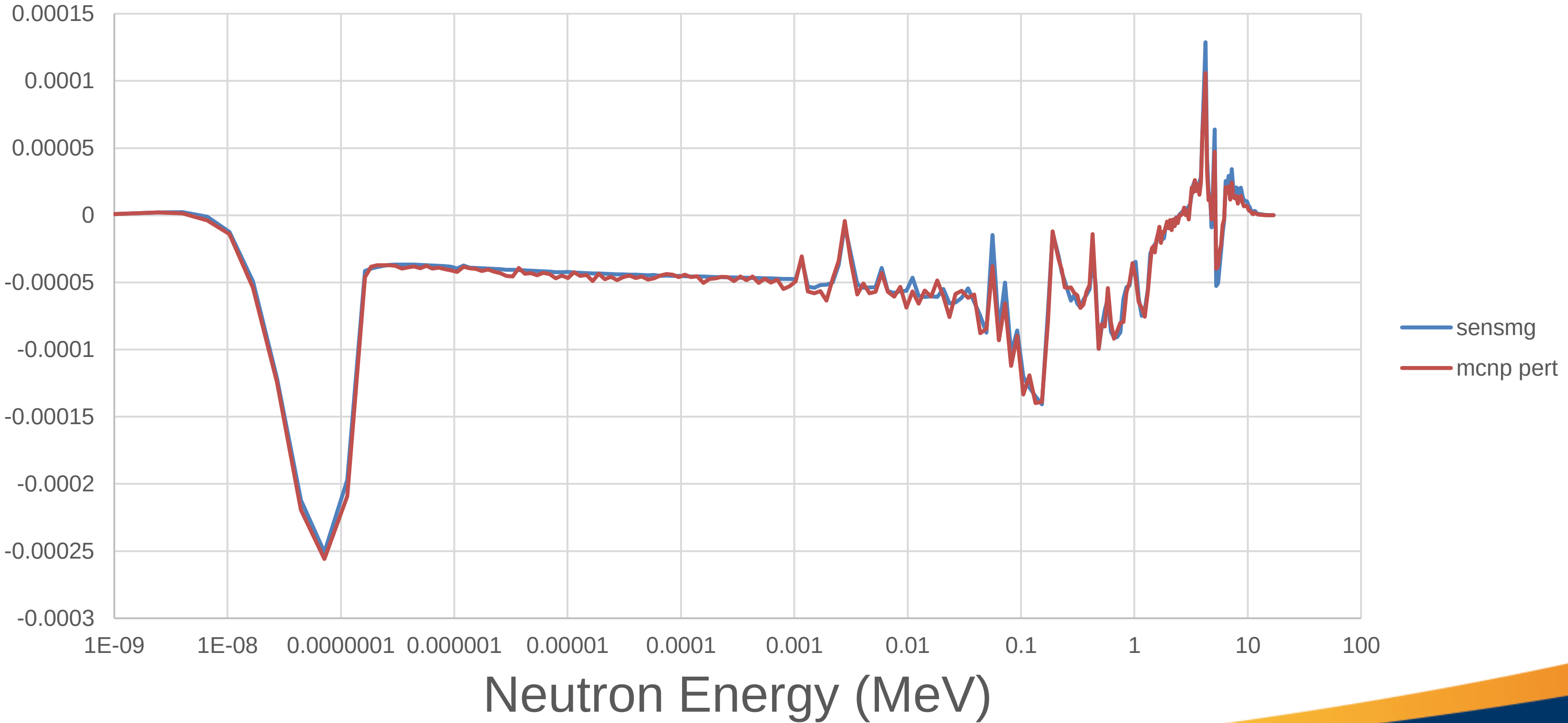
O16 Sensitivities (% delta leakage / % delta xs)
P0+P1+P2+P3 versus MT's 2,4,16,22,23,28
(fission source inside a 6" radius concrete sphere)



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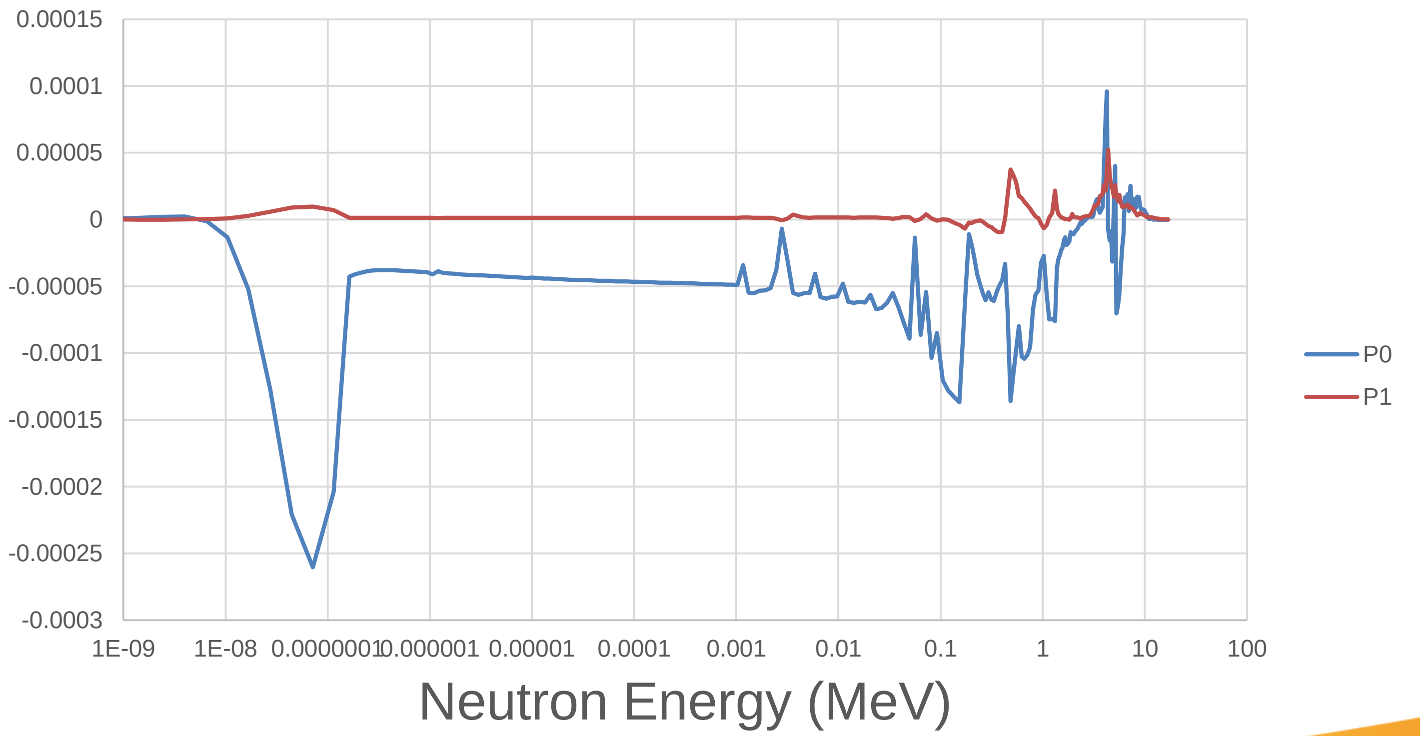
O16 Sensitivities (%delta leak / %delta xs) (Fission Source in a Concrete Sphere)



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A Sandwich Rule Result from JENDL 4.0 O-16 mubar Uncertainties on a Concrete Sphere

- JENDL 4.0 mubar covariance data for O-16 was processed in NJOY and a relative covariance matrix was generated (also MT 2 – elastic scattering)
- P0, P1, and PL Sensitivity vectors for the leakage from the sphere were generated with SENSMG and MCNP using ENDF/B VII.1 data
- Assumption:
  - Elastic Scattering off of O-16 dominates inelastic or (n,xn) reactions in the sensitivity vector calculation

Covariance Data	Sensitivity Vectors	Number of Groups	Leakage Sens. (%/%)
mt 2 JENDL 4.0	P0 ENDF/B VII.1	250	8.701e-5
mt 2 JENDL 4.0	PL ENDF/B VII.1	250	8.710e-5
mf 34 JENDL 4.0	P1 ENDF/B VII.1	250	3.994e-5

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A Sandwich Rule Result from ENDF/B VIII.0 Pu-239 mubar Uncertainties on Jezebel

- ENDF/B VIII mubar covariance data for Pu-239 was processed in NJOY and a relative covariance matrix was generated
- P1 Sensitivity vectors for Jezebel were generated with SENSMG using ENDF/B VIII data (or ENDF/B VII.1)
- Assumption: Elastic Scattering off of Pu-239 dominates inelastic or (n,xn) reactions in the sensitivity vector calculations

- ~160 pcm (0.00160 in k_{eff}) was the estimated overall uncertainty due to mubar – in either 30g or 250g analysis
- Comparable in magnitude to the “official” cross section (total, elastic, inelastic, fission, capture, nubar, and fission spectrum) uncertainties for Jezebel as given in the CIELO / ENDF/B VIII release paper. The official values range from ~30 pcm and ~900 pcm.

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Summary

- Overall Uncertainty = Covariance Data * Sensitivity
- *"It was found that in the case of small systems with large leakage effects, such as JEZEBEL Pu239, the sensitivities due to mubar, are non-negligible and contribute relevant uncertainties. … It was also noted that, as expected, the mubar sensitivities are mainly distributed in the high energy range." (from a 2012 paper by Aliberti and McKnight)*
- mubar uncertainties should be included with the other uncertainties in the analysis of systems like Jezebel and Godiva

Future Work

- Continue fixing the O-16 mubar covariance data in ENDF/B VIII
  - Group T-2 at Los Alamos
- Extend NJOY to handle alternate MF 34 MT 2 formats (e.g., for U-235 mubar)
  - Nuclear Data Team at Los Alamos
- Extend evaluated covariance data and NJOY processing to P2, P3, etc
  - Anyone?, NJOY team?
- Extend SENSMG to include the individual cross sections which are currently mixed together in the Legendre “scattering” blocks
  - Work with Jeff Favorite of Los Alamos

- In future ENDF/B work on standard problem (e.g., Jezebel, Godiva) uncertainties, include mubar!
  - CSEWG and the ENDF community

Extra Slides

2012 Published Result: Trans ANS, 107, p.1093 by Aliberti and McKnight

- *"It was found that in the case of small systems with large leakage effects, such as JEZEBEL Pu239, the sensitivities due to mubar, are non-negligible and contribute relevant uncertainties. … It was also noted that, as expected, the mubar sensitivities are mainly distributed in the high energy range."*

Their multi-group study used an arbitrary 10% uncertainty on mubar by changing both the P1 elastic scattering cross sections for self- and down-scattering by 10%. (There was no up-scatter in their problems, and there was only 1 down-scatter group.)

- 2013, Trans ANS, 109, p. 735, Kiedrowski obtained similar results for 10% Uncertainty in mubar in multi-group Monte Carlo calculations.

Where does the mubar covariance data live in the ENDF Evaluation data?

- In ENDF 6 formats, elastic scattering cross sections are found in mf 3 mt 2, and elastic scattering outgoing angular distributions are found in mf 4 mt 2. By convention, covariance data is placed in mf + 30.
- Covariance data for elastic scattering cross sections are in mf 33 mt 2, while the mubar covariance data is found in mf 34 mt 2.
- Just like cross section covariance data from mf 33 is processed by NJOY into multi-group covariances, mubar covariance data from mf 34 is processed by NJOY into multi-group data
  - NJOY modules Errorr, Covr, and Viewr are used to process the data
  - “mfcov” on card 7 is the relevant option

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Covariance matrix basics

- A covariance matrix is symmetric
- A covariance matrix is positive (or semi-positive) definite
  - All eigenvalues are positive (or at least non-negative)
  - In our single precision world, we do allow small negative “round-off” eigenvalues as long as they are close to 0.0. (say -1.0e-10)
  - Canned software packages may not handle these “round-off” eigenvalues
- The associated **correlation** matrix should have all values bounded between -1 and +1 and also values of +1 on the diagonal. *(absolute covariance matrix (i,j) and stdev's (i), (j))*
- For my application into the “sandwich” rule, the **relative covariance** matrix is also required. *(absolute covariance matrix (i,j) and mean values (i), (j))*
- For real life applications, the variances (and stdev’s) should be bounded – i.e., <u>not larger</u> than the valid range of values (-1 to +1) for mubar

Covariance Data for the Sandwich Rule

- I use the "Relative Covariance" matrix
  - Relative Covariance Matrix (i,j) = Absolute Covariance matrix(i,j) / Mean(i) / Mean(j)
- Relative Covariance is NOT the same as Correlation
- Relative Covariance is resistant to numerical round-off errors

- Covariance data is problem independent
  - Depends only on the cross sections and properties of the isotopes …

- Covariance data is given in the nuclear data evaluation file
- NJOY is used to generate multi-group covariance data
  - ERRORR, COVR, and VIEWR modules
  - "mfcov" on card 7 of ERROR

How about those (very small) negative eigenvalues in the covariance matrix?

Two Approaches:

- Assume the (very small) negative eigenvalues are 0.0 and only use the positive eigenvalues for replica data generation

- There is an alternative method:
  - “ridge correction” – add a small epsilon along the diagonal of the covariance matrix – thereby shifting all eigenvalues up in value by the small epsilon amount
    - Does not really change the big eigenvalues and their eigenvectors very much
    - Does change the “very small” and small eigenvalues and their eigenvectors significantly

A typical set of 30 eigenvalues:

0.0012139	1.7779E-09
0.00051391	0
0.00014548	0
0.00003267	0
0.000013658	0
9.4226E-06	0
3.9759E-06	0
5.7225E-07	0
9.5012E-08	0
5.4728E-08	0
4.8051E-08	-2.5856E-12
4.0415E-08	-2.1816E-10
2.6692E-08	-5.9191E-09
1.3939E-08	-1.6388E-08
7.03E-09	-5.5935E-08

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Two Approaches for Uncertainty Analysis

- For Steady State (say k_{eff})
- Use Relative Covariances in the Sandwich Rule with the Sensitivity Vectors (% / %)
- Multiply the Sandwich Rule out and get the output parameter variance or standard deviation.

- For Dynamic Situations
- Use Absolute Covariances to generate replica data (> 75x)
- Run the calculation with each set of replica data
- Accumulate statistics to measure the output parameter's variance or standard deviation.

Sandwich Rule Multiplication

- resultant variance / (output quantity)^2 = [Sens]^T * [Covariance] * [Sens]

- Where [Sens] is a vector of sensitivities (problem specific)
  [Cov] is a covariance matrix (inherent data)

- Practical Advice #1: Be very sure the group orderings are consistent
  - NJOY is Low E to High E
  - MCNP is Low E to High E
  - SENSMG and Partisn are High E to Low E
- Practical Advice #2: Be very sure that your units work out between “Sens” and “Covariance”

- The result is the variance/output^2 due to (1) the uncertainties in the input parameter data and (2) the sensitivities of the output for the problem at hand due to a change in the input parameters.
- The square root of variance/output^2 is the relative standard deviation (stdev/output)

Generating Replica Data for Uncertainty Analysis

- Use the absolute covariance matrix
- Usually work with multi-variate normal random number generators to generate correlated random samples
  - Relative uncertainties above ~43% will produce some (~1%) negative samples from a Gaussian distribution
  - Preserving non-negativity due to large uncertainties might necessitate log-normal distributions
- As an aggregate whole, the replica data (~75x or more) should/must
  - Preserve the mean values
  - Preserve the variance/stdev values on the mean (i.e., the diagonal elements)
  - Preserve the covariance values (i.e., the non-diagonal elements)
- BTW, there is a method available to preserve all these aggregate quantities EXACTLY for “n” samples
  - Uses renormalization for the means and a singular value decomposition method for the covariances
  - All “n” samples must be used – no more and no less
  - Why do statisticians not like this? *I do not know …* It is available as an option in “R”, a statistics programming environment – where it is called “preconditioning” (the empirical = “T” option) in the mvrnorm R routine
- If “n” is very large, then the normal statistics are nearly converged and the quantities are nearly preserved
- Run the calculation for each set of replica data – ideally ~75x or more
- Accumulate statistics from the output quantities of interest from each replica calculation
  - Measure the variances (or stdev) of the output quantities of interest
  - Do an analysis of variance if multiple input parameters were changed at the same time

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Allocating the delta mubar to all of the outgoing energy groups

- NDI Tables have a “ 1 “ (for P1) section after the “ 0 “ (for P0) section in the “pn_full” data after the “pn_order” (the number of Legendre scattering orders, typically 5)
- **Make the replica mubar data by modifying the P1 scattering cross sections**

- Remember -1 ≤ μ(i,j) or mubar(i) ≤ 1 is still required
- Also try to preserve the monotonicity that **usually** is present in multi-group scattering data (μ(i,j))
  - Self-scattering is forward peaked
  - Down-scattering is more and more backward peaked as the neutrons scatter further and further down in energy

- Arbitrary selection of allocation methods – so long as the overall sums of outgoing group cross sections (P1/P0) preserve mubar
  - Could split evenly (say 10% of the delta mubar into each of 10 outgoing groups)
  - I use the fraction of the individual P0 xs / sum of all P0 xs to allocate the change in mubar to the μ’s and generate the new P1 xs – with ad hoc adjustments as needed to satisfy the required constraints

An approximate way to estimate O-16 mubar effects …

Compare O-16 from ENDF/B V and VIII

(Credit Pete Jaegers for this idea.)

- Elastic scattering is almost the only reaction for O-16
- O-16 elastic scattering is nearly identical between V and VIII
- Only the mubar data is different