Monte Carlo Based Uncertainty and Sensitivity Analyses at LANL

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Abstract

- Recent uncertainty and sensitivity analysis work at LANL is reviewed. Monte Carlo analysis methods are described. The cross section uncertainties studied so far include σ_f, χ, and σ_{n2n}. Random sampling methods are used to generated correlated normally distributed replica cross sections. The replica cross sections are used in partisn to calculate the distribution and uncertainty of output parameters like k_{eff}. Sensitivity analysis methods are also described. Additionally, constraints on cross section covariance matrices are discussed and illustrative examples are given. Finally, some details of recent LANL results with fission spectrum uncertainty are presented.

Talk Overview

- Overview of Monte Carlo based Uncertainty and Sensitivity Analysis
- Constraints of the Covariance Matrices
- LANL Work with Fission Spectrum Uncertainties

Overview of LANL Work

- **In contrast to deterministic methods of uncertainty and sensitivity analysis, we at LANL have used Monte Carlo methods of uncertainty and sensitivity analysis for several years.**
- **First Paper: T. Kawano, et al, "Evaluation and Propagation of the ^{239}Pu Fission Cross-Section Uncertainties Using a Monte Carlo Technique", NSE, Vol. 153, pp. 1-7, (2006)**
  - Demonstrated the use of an integral constraint (Jezebel k_{eff}) to modify both the fission xs and also the covariance matrix of the fission xs.
- **We have focused on the uncertainties in fission xs, fission spectra, and n2n xs and their effects on the uncertainties in output quantities like k_{eff} and reaction rates**
- **We are currently investigating cross section uncertainties which include reaction to reaction cross correlations in 30 groups (hopefully 618 in the future)**
  - Total, elastic, inelastic, n2n, n3n, fission, and capture reactions included
  - Strong correlations exist between different reactions

Monte Carlo Based Uncertainty Analysis (Direct Approach)

- **Given: nominal group-wise values of the xs of interest and their covariance matrix (or standard deviations for each xs and a correlation matrix)**
- Assume a normal distribution for each of the input xs values
- Generate "replica" xs data, i.e., multivariate normal samples of the input xs or spectrum of interest
  - The replicas, as an aggregate whole, must closely reproduce the given nominal values for the xs or spectrum and the given covariance matrix
  - Standard methods exist to generate these correlated random samples
- Run the code calculation (e.g., partisn) for each of the replica sets of input data
- Accumulate output parameter statistics (e.g., the standard deviation of the k_{eff} results)

Our Method of Statistical Sampling (assume normal distribution for input parameters)

- **Decompose the (positive definite) Covariance Matrix into (positive) eigenvalues and associated eigenvectors**
  - Algebraically equivalent to diagonalizing the covariance matrix
- **Sample the variations of each of the parameters from a normal distribution using their given means and standard deviations**
  - Log normal distributions may be used to prevent negative values
- **Multiply the eigenvectors by their sampled eigenvalues and add eigenvectors all back together**
  - If eigenvectors are not used, correlations/covariance will NOT be preserved
- **Alternative methods are available to generate these correlated random samples:**
  - Cholesky Decomposition – but does not allow PCA type approaches
  - Matrix square roots – but does not allow PCA type approaches
  - Singular Value Decomposition
- **Standard statistical routines are available for multivariate normal distributions**
  - MATLAB has "mvnrnd"
  - R has "mvrnorm" and optionally includes "pre-conditioning"

What if the Covariance Matrix isn't Positive Definite?

- **Any eigenvalues = 0.0 indicates missing degrees of freedom (or incomplete information or some other constraint) – OK**
  - Covariance Matrix is still semi-positive definite
- **Any eigenvalues very near to 0.0 may be round-off error– probably OK, but canned subroutines will fail, --- use locally developed extensions**
- **Any eigenvalues significantly < 0.0 or complex indicates errors in the covariance matrix – NOT OK**

More Sophisticated Statistical Approach (with the help of Group CCS-6 at LANL)

- **Given: nominal groupwise values of the xs of interest and the covariance matrix (or standard deviations for each xs and a correlation matrix)**
- Sample "uniformly" (e.g., Latin hypercube) throughout the multi-dimensional input parameter phase space (to say, +/- 3σ) and run the samples through the original code
- Generate a code surrogate – (using a Gaussian Process Model) – with the sample inputs and code outputs from these "training runs"
- Obtain the output uncertainties
- Obtain the sensitivities using a "main effect" and a "total effect" breakdown from the analysis of variance
  - "total effect" accounts for interactions between input parameters

Details of the partisn calculations of Jezebel (Similar model exists also for Godiva)

- **30, 250, or 618 groups LANL data**
- **250 mesh cells (over ~6.5 cm)**
- **1D spherical geometry**
- **S_{48} quadrature and P_3 xs**
- **Diagonal transport correction applied**
- **1e-7 convergence criterion**

- ***The idea is to have a very well converged 1D solution.***

Deterministic versus Monte Carlo Uncertainties (wrt Jezebel and Godiva k_{eff}'s)

- Following the Review Papers of Cacuci and Ionescu-Bujor, "A Comparative Review of Sensitivity and Uncertainty Analysis of Large-Scale Systems …", NSE, Vol. 147, pp. 189-203 and 204-217, (2004):
- Using 30, 250, and 618 groups, we generated the k_{eff} output uncertainty of Jezebel and Godiva k_{eff}'s based on the given input uncertainties for Σ_f:
- Deterministic (a la ANL)
  - We estimated the group-wise sensitivity vector elements (Δ k / Δ fission xs) by a series of partisn calculations of Jezebel wherein one and only one individual group fission xs was perturbed by +/- 0.5 %
  - Output k_{eff} uncertainties were calculated from the "sandwich rule"
    - **$S\ V\ S^T$**, where V is the covariance matrix of the fission xs and S is the sensitivity vector
    - ***Correlation effects are thus included in the output uncertainty***
- Monte Carlo (a la LANL)
  - Use covariance matrix to generate replica fission xs data
  - Run partisn (or a partisn emulator) with each set of replica data
  - Accumulate output statistics to "measure" output uncertainty
  - ***Correlation effects are thus included in the output uncertainty***
- **Identical Output Uncertainty Results were obtained (within statistical noise)**

Godiva and Jezebel k_{eff} Uncertainty Results (stdev of k_{eff} caused by Σ_f uncertainty)

	30 Group	250 Group	618 Group	30 Group	250 Group	618 Group
	Det.	Det.	Det.	MC	MC	MC
Godiva "before"	0.403 %	0.326 %	0.326 %	0.407 %	0.327 %	0.327 %
Godiva "after"	0.097 %	--	0.096 %	0.098 %	--	0.095 %
Jezebel "before"	0.467 %	0.261 %	0.261 %	0.463 %	0.259 %	0.260 %

Monte Carlo Based Sensitivity Analysis

- **The question to be answered is how important is (the uncertainty of) each input parameter with respect to the uncertainty of a given output parameter**
- **So far, we have relied on simple methods of sensitivity analysis – like linear correlation coefficients – between input and output parameters**
  - Assumes linear variations
    - Rank correlation coefficients should handle mild to moderate non-linearity
  - Assumes independent input parameters
- **For fission spectrum work, a composite input parameter (either the average velocity or the average energy of the sampled fission spectra) looks very promising for sensitivity analysis.**
- **(Future work) How do we address sensitivity when the inputs are non-linear and or correlated?**

Constraints on Covariance Matrices

- **For Fission Spectra Covariances**
  - The Constraint is the normalization to 1.0
  - Use the **zero sum rule** for rows and columns of the absolute covariance matrix
  - One of the eigenvalues of the covariance matrix will be zero
- **For Cross Section Covariances (involving Σ_{total} and its components)**
  - The Constraint is that $\Sigma_{total} = \Sigma_{elastic} + \Sigma_{inelastic} + \ldots$
  - **Proposed new rule**: (assume the first row and column represent Σ_{total})
    - (for each group)
    - For every column: the first row covariance = the sum of the other entries
    - For every row: the first column covariance = the sum of the other entries
  - One of the eigenvalues of the covariance matrix will be zero

Sample Covariance Matrix for Fission Spectra (Zero Sum Rule)

1.0	-0.3	0.2	-0.6	-0.3
-0.3	1.0	-0.3	0.1	-0.5
0.2	-0.3	1.0	-0.6	-0.3
-0.6	0.1	-0.6	1.0	0.1
-0.3	-0.5	-0.3	0.1	1.0

- **Each row (or each column) corresponds to a group**
- **All rows sum to 0.0**
- **All columns sum to 0.0**
- **Eigenvalues = 2.139, 1.5, 0.8, 0.5610, and 0.0**
- **Thus, this matrix is semi-positive definite**
- **The first 4 eigenvectors (those with a non-zero eigenvalue) also have elements which sum to 0.0**
- **Thus the correlated sampling scheme will preserve the desired chi normalization**

Proposed Criterion for Covariance Matrices with Cross Section Balance

- **Cross Section Balance means (total xs) = (elastic xs) + (inelastic xs) + (n2n xs) + (n3n xs) + (fission xs) + (capture xs) for each group**
- **Analogous to the zero sum (or zero column) rule for fission spectra covariance matrices, we propose a sum rule (or column rule) for covariance matrices which require cross section balance:**
- **Cov(total xs) = Cov((elastic xs) + (inelastic xs) + (n2n xs) + (n3n xs) + (fission xs) + (capture xs))**
- **The inherent assumption is that we know the total xs exactly, whereas we really know it only to fairly tight precision,** *but we do know it better than all of the rest of the xs.*
- **Checking this on some NJOY generated 30 group xs for Pu-239 (with most cross terms included for 7 reactions) showed that the higher energy groups satisfied this rule while the lower energy groups did not**

Sample Matrix for Proposed New Rule for Covariance Matrices with Cross Section Balance

1.0	0.1	0.2	0.5	0.2
0.1	1.0	-0.4	-0.3	-0.2
0.2	-0.4	1.0	0.0	-0.4
0.5	-0.3	0.0	1.0	-0.2
0.2	-0.2	-0.4	-0.2	1.0

- **Row and Column 1 represent the total xs**
- **The other rows and columns represent the component parts of the total xs**
- **For all rows, the first column = the sum of the rest of the columns**
- **For all columns, the first row = the sum of the rest of the rows**
- **Eigenvalues = 1.681, 1.360, 1.161, 0.7978, and 0.0**
- **Thus, this matrix is semi-positive definite**
- **The first 4 eigenvectors (those with a non-zero eigenvalue) have elements which also satisfy the constraint given above**
- **Thus the correlated sampling scheme will preserve the desired xs balance**

Two Methods of Fission Spectrum Uncertainty and Sensitivity Analysis

- **The Four Parameter Approach**
  - Uses 4 parameters of the Madland-Nix Formula
  - Chi Normalization by PFNS code
  - Preferred Solution
- **The Direct Fission Spectrum Approach**
  - Uses tables of actual chi data at several hundred energy points
  - Normalization by the “zero-sum” rule for covariance
  - Useful for Consistency Checking
- **Both methods use a chi vector (not a chi matrix) with an average incident neutron energy = 0.5 MeV**

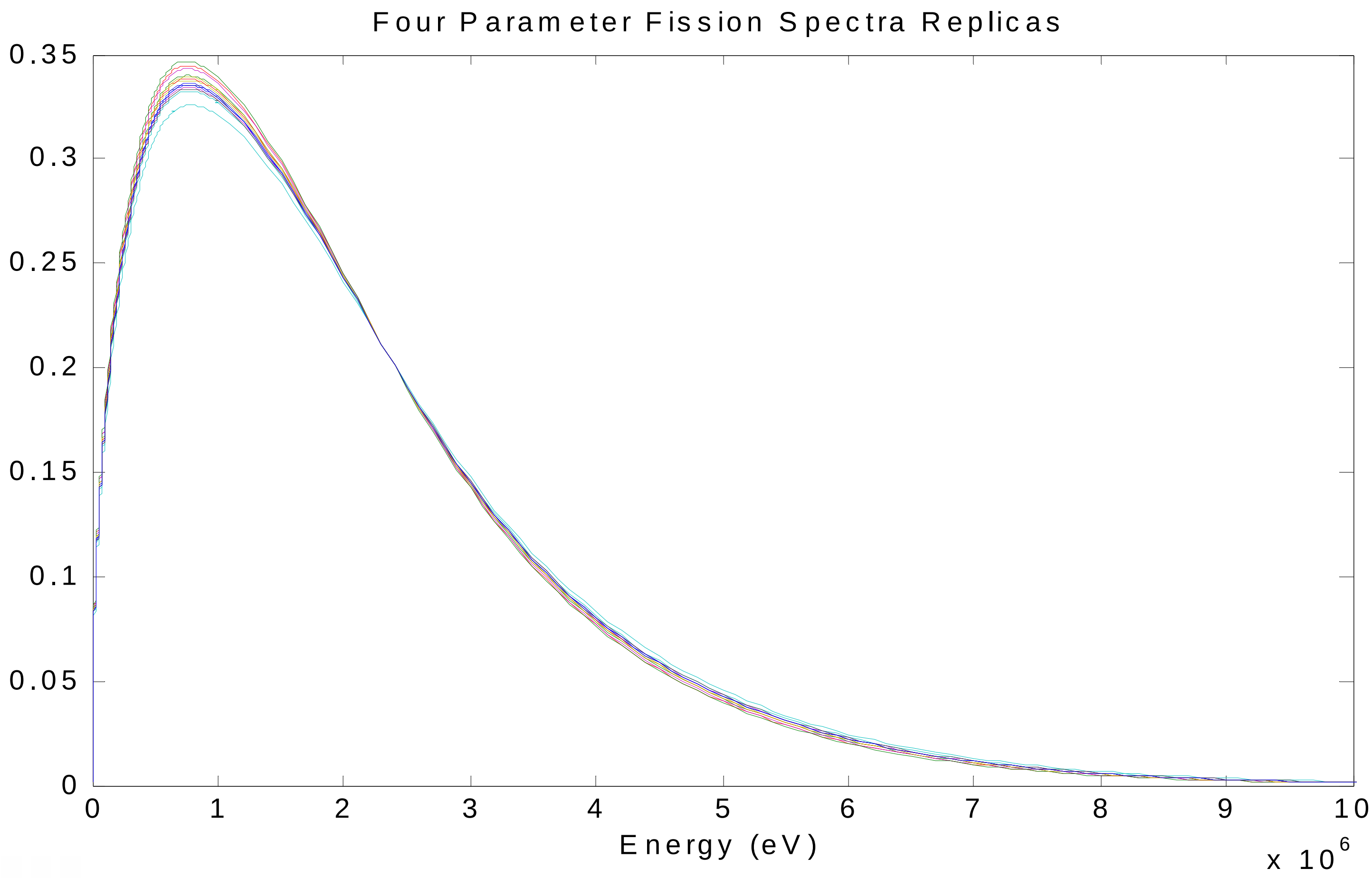
Sampling of the Four Parameters (E released, TKE, B_n, Level Density)

- **Given: Nominal Values of Each Parameter and also its Standard Deviation and the 4x4 Correlation Matrix (ie Covariance)**
  - Assume input variations are “normal”
- **Use standard statistical sampling techniques to generate replica sets of the Four Parameters**
  - The 4x4 matrix is positive definite
  - The replicas (as a aggregate whole) will “preserve” the means, standard deviations, and correlations which were specified

Correlation Matrix of the Four Parameters for PFNS

	Energy Released	Total Kinetic Energy	Neutron Binding Energy	Level Density
Energy Released	1.000	0.823	-0.090	0.374
Total Kinetic Energy	0.823	1.000	0.043	-0.181
Neutron Binding Energy	-0.090	0.043	1.000	0.018
Level Density	0.374	-0.181	0.018	1.000

Four Parameter Replica Fission Spectra for Pu-239 (at 0.5 MeV incident energy)



Propagating the Four Parameter Replica Data

- **Given: replica sets of the Four Parameters**
  - E released, TKE, B_n, Level Density
- **Use Madland-Nix Formula in PFNS code to generate a fission spectrum for each replica set of parameters**
  - Chi normalization handled by PFNS
- **Allocate fission spectra into multigroup energy structure**
- **Repeatedly run (~1000x) the multigroup Sn code analysis of interest and accumulate output results**
- **Analyze the output results for means, standard deviations, etc. (Uncertainty Analysis)**
- **Compare input data with output replica results (Sensitivity Analysis)**

Direct Sampling of the Fission Spectrum

- **Given: Nominal Chi Values at several hundred energies and also their Standard Deviations and the large Correlation Matrix (ie Covariance)**
  - Usually assume input variations are "normal"
  - May need log-normal to prevent negative values
- **Chi normalization preserved by "zero-sum" rule applied to the large covariance matrix**
- **Use standard statistical sampling techniques to generate replica chi spectra**
  - The large matrix is ~ semi-positive definite
  - The replicas (as a aggregate whole) will "preserve" the means, standard deviations, and correlations which were specified

Propagating the Replica Fission Spectrum Data

- **Given: replica sets of the fission spectrum each with several hundred energy points**
  - Normalization was preserved by the “zero-sum” rule
- **Allocate fission spectra into multigroup energy structure**
- **Repeatedly run (~1000x) the multigroup Sn code analysis of interest and accumulate replica output results**
- **Analyze the output results for means, standard deviations, etc. (Uncertainty Analysis)**
- **Compare input replica data with output results (Sensitivity Analysis)**

Jezebel Analysis with Fission Spectrum Uncertainty

- **Canonical measured k_{eff} uncertainty = 0.0020**
- **Earlier high/low bracketing gave k_{eff} uncertainty ~ 0.0036 for LANL, ~ 0.0048 for LLNL, for the 1 Sigma changes in chi**
- **Current estimate (based on 1000 Jezebel runs) of k_{eff} uncertainty due to fission spectrum uncertainty = 0.0024**
  - Uses Four Parameter Approach
  - Direct Approach result = 0.0020

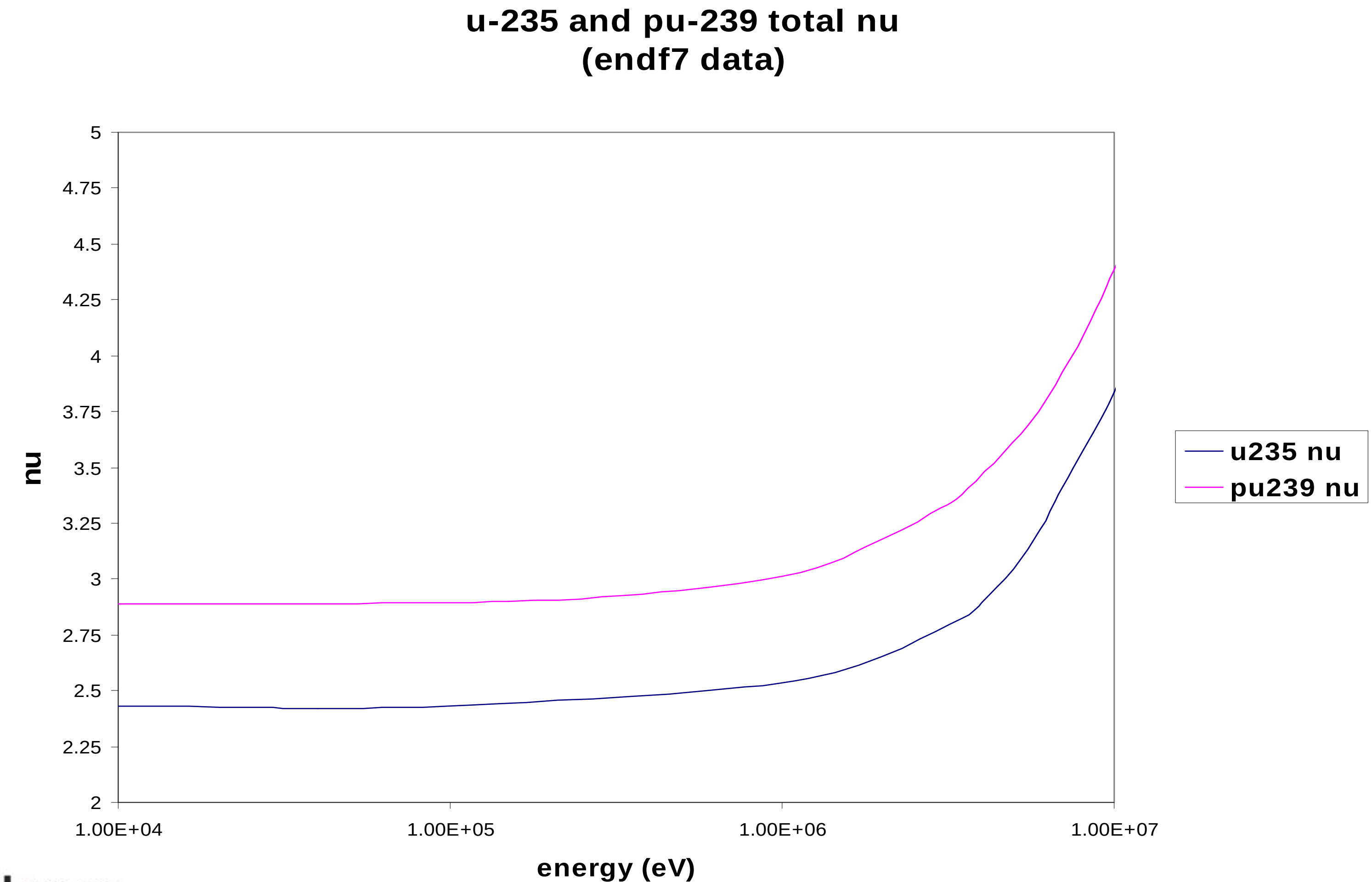
Approximate Sensitivity Analysis of Jezebel Results

- **Simple linear correlation coefficient analysis used to estimate relationships between input parameters and output results**
- **Two promising composite input parameters are also being investigated for future work – the average energy and the average velocity of the replica fission spectra. (thanks to John Lestone and Jeff McAninch)**

Approximate Sensitivity of Jezebel k_{eff} to the input parameters

Input Parameter	Linear Corr. Coef. wrt to k_{eff}
Energy Released for PFNS	-0.5257
Total Kinetic Energy for PFNS	0.7421
Neutron Binding Energy for PFNS	0.1455
Level Density for PFNS	-0.9840
Average Chi Energy	1.0000
Average Chi Velocity	0.9999

Why might the averaged Energy or Velocity from the fission spectrum matter so much to k_{eff}?



Summary

- Overview of Monte Carlo based Uncertainty and Sensitivity Analysis being carried out at LANL
- Insightful comparisons with deterministic methods
- Question about Sensitivity Analysis when the input parameters are correlated
- Proposed Covariance Matrix constraint for XS with Σ_{total} and its component parts
- Four Factors of the Madland-Nix formula used in Fission Spectrum Analysis (as opposed to a direct approach using groupwise χ values)