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Preliminary Covariance Data Representation for the "A Compact ENDF" File

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Abstract

Modifications to the the A Compact ENDF (ACE) format for convariance data is proposed. The format represents the covariance matrices with principal eigenvectors, which allows for significant data compression. The results from keff uncertainty calculations for ICSBEP benchmark experiments are acceptable, demonstrating that significant memory savings is possible.

Overview

- Motivation and Background
- Format Description
- Results

Motivation

- **Perform uncertainty quantification of calculated responses from simulation software**

- **Sources of uncertainty:**
  - **Geometric tolerances, material compositions, nuclear data, Monte Carlo random process, etc.**

- **Linear estimate of uncertainty in a response:**

$$\delta k^2 = \bar{\mathbf{S}}\,\bar{\bar{\mathbf{C}}}\,\bar{\mathbf{S}}^T$$

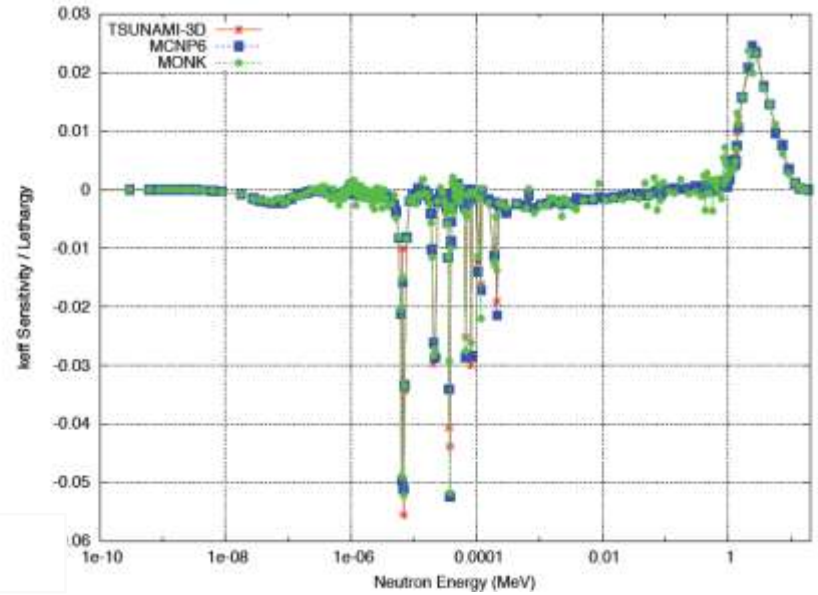
S = sensitivity vector (response derivatives w.r.t. system parameters)

C = covariance matrix of system parameters

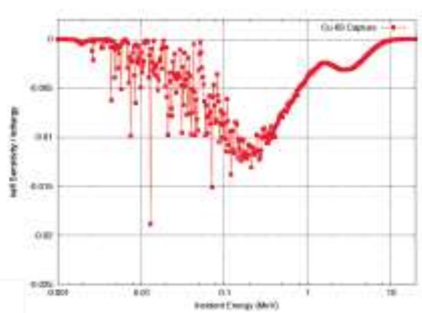
Sensitivity Vector from MCNP

- **MCNP6 can produce sensitivity coefficients to *k* in continuous-energy**
  - Uses adjoint-weighted perturbations
  - Computes sensitivity coefficients for cross sections, fission, & scattering laws.
  - User-defined energy resolution for results or tallies – no discretization
  - Nuclear Science & Engineering paper accepted and in publication (July 2013)
  - Can directly compare to TSUNAMI multigroup S/U results

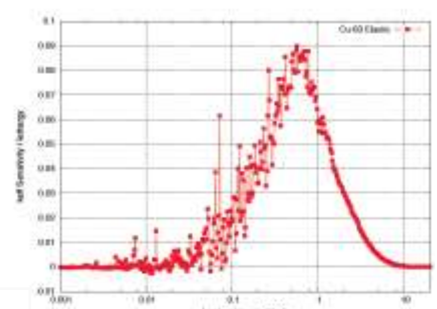
MOX Lattice: U-238 Total



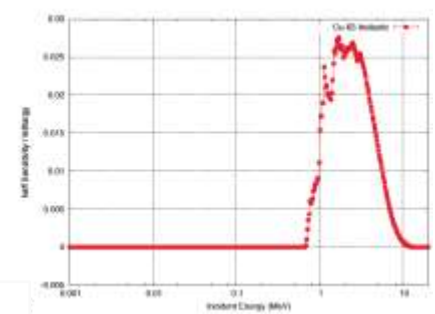
Zeus: Cu-63 Capture Cross-Section Sensitivity



Zeus: Cu-63 Elastic Cross-Section Sensitivity



Zeus: Cu-63 Inelastic Cross-Section Sensitivity



MCNP6 Sensitivity User's Guide on MCNP website: LA-UR-13-22251.

Covariances

- **Covariances are in the ENDF file, but this is never accessed by MCNP, which reads the ACE file processed by NJOY**
  - **Need a means for MCNP to obtain the covariances**

- **Options:**

  1) Prepare a special file for MCNP to read

  2) Modify the ACE format and NJOY to incorporate covariances

- **Selected option 2, modify ACE and NJOY**
  - **Easier to incorporate into data processing workflow**
  - **Less impact on the old, inflexible routines in MCNP that process cross sections**

ACE Covariance Format

Design Considerations

- **Covariance data may be represented as a symmetric matrix for the overall system**
  - **All isotopes, reactions, energies correlated with each other**
- **Large amount of data (100's MB to GB required for raw data)**
  - **Upper triangular representation (easy, lots of data)**
  - **Compressed upper triangular (trickier, some savings)**
  - **Principal eigenvectors (most difficult, most savings)**
- **Principal eigenvector format selected**
  - **Most practical for long term considerations of memory (RAM) and data distribution**

Principal Eigenvectors

- **Covariance matrix may be decomposed into eigenvalues and eigenvectors:**

$$\bar{\bar{\mathbf{C}}} = \bar{\bar{\mathbf{V}}}\,\bar{\bar{\mathbf{D}}}\,\bar{\bar{\mathbf{V}}}^{T}$$

V = Matrix of column of eigenvectors

D = Diagonal matrix of corresponding eigenvalues

- **The covariance matrix may often be reproduced to sufficient accuracy with a much smaller subset of eigenvectors and eigenvalues**
  - **Take N largest eigenvalues and corresponding eigenvectors**
  - **Large memory savings often possible for many data sets**

Principal Eigenvectors

- **Magnitude of an eigenvalue describes the amount of variability along a particular eigenvector direction**
  - Eigenvectors with largest eigenvalues should be able to capture most of the variability
- **Define a residual:**

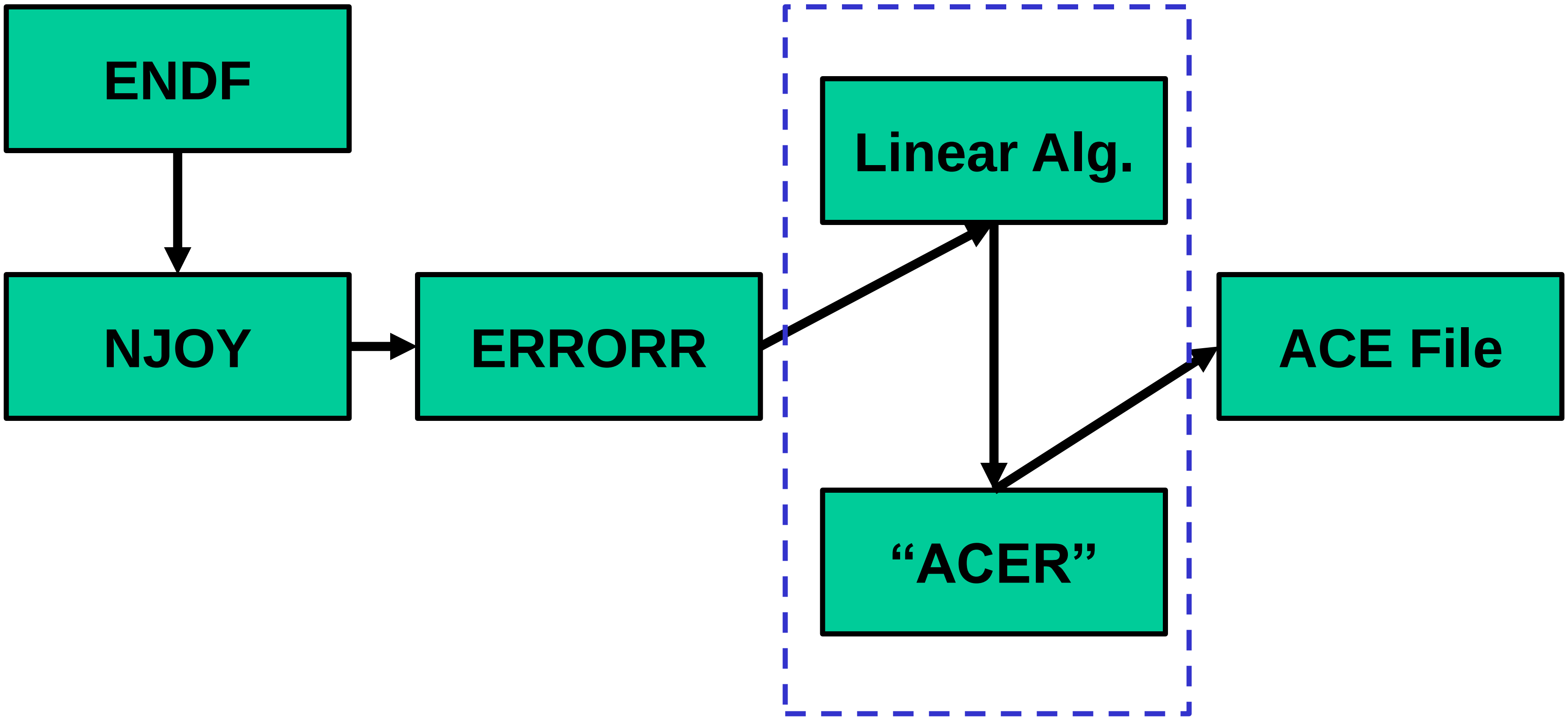
$$R = 1 - \frac{g_N}{g}$$

g = sum of positive eigenvalues

g_N = sum of first N positive eigenvalues

- **Assign N based on user parameter *R*.**
  - **Choose *R* so that uncertainty estimates are accurate**
- **Note: some eigenvalues may be negative because of single precision representation in ENDF.**

Workflow Diagram



Insert these routines into NJOY eventually

ACE Covariance Format

- **Separate data block for each table, which may contain many covariance matrices.**

- **Includes:**
  - **Link to next covariance matrix, if any**
  - **Header**
  - **List of isotopes and reactions**
  - **Unionized energy grid**
  - **Eigenvalues**
  - **Eigenvectors in compact representation (zeroes excluded)**

- **Loaded into XS arrays in MCNP, and covariance matrix elements are computed as needed to limit memory requirements.**

MCNP Prototype

- **Special version of MCNP reads new ACE format, generates sensitivity profiles, and convolves them to produce uncertainty estimates**
  - **Example output for ENDF/B-VII.1 Pu-239 in Jezebel:**

94239.80c	elastic	elastic	462.1
94239.80c	elastic	inelastic	-867.5
94239.80c	elastic	n,2n	-3.4
94239.80c	elastic	fission	-82.2
94239.80c	elastic	n,gamma	36.0
94239.80c	inelastic	inelastic	859.0
94239.80c	inelastic	fission	1.3
94239.80c	n,2n	n,2n	11.1
94239.80c	fission	fission	331.0
94239.80c	fission	n,gamma	0.3
94239.80c	n,gamma	n,gamma	72.4
94239.80c	total nu	total nu	81.6
94239.80c	fission chi	fission chi	174.1
94239.80c			587.6

Results

Results

- Generate covariance data for major actinides (U-235/238 and Pu-239) and try computing uncertainties in benchmarks.

- Error estimate:

$$E = 1 - \frac{\delta k_N}{\delta k}$$

  - Compares to that obtained by N eigenvalues to reference obtained with all eigenvalues.

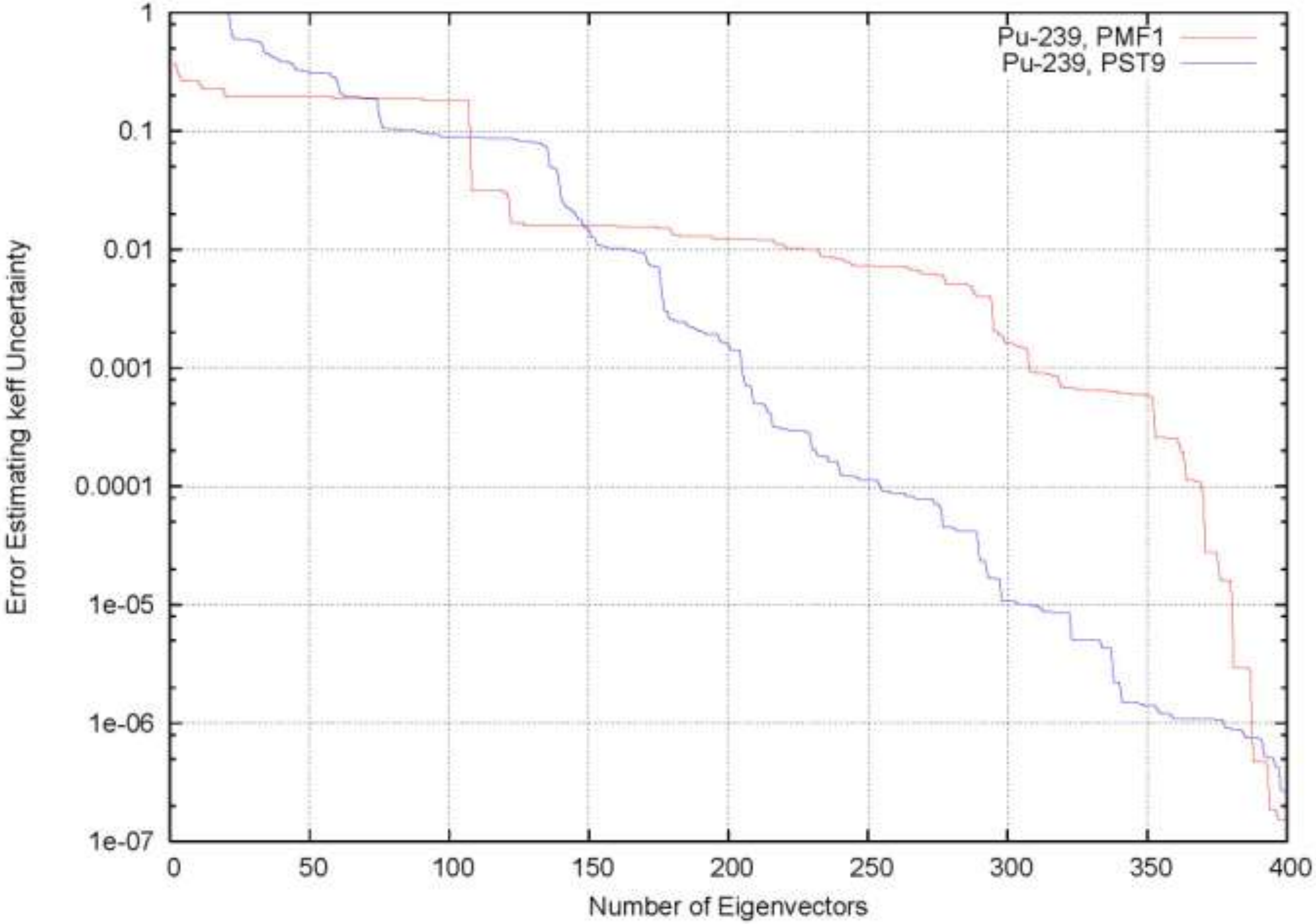
- Correlate with residual to see if user parameter for generating data can be set conservatively

Pu-239

- **Covariance data**
  - **Reactions: total, fission, elastic, inelastic, capture, (n,2n), (n,3n), (n,4n)**
  - **Energy groups: 476**
  - **ERRORR File Size: 18 MB**
- **Benchmarks**
  - **Jezebel (Pu-MET-FAST-001)**
  - **Plutonium Solution (Pu-SOL-THERM-009)**
- **Maximum error *E* versus percent memory savings *S*:**

E	**10^{-2}**	**10^{-3}**	**10^{-4}**	**10^{-5}**
***S* (Pu-239)**	**80%**	**73%**	**67%**	**67%**

Pu-239

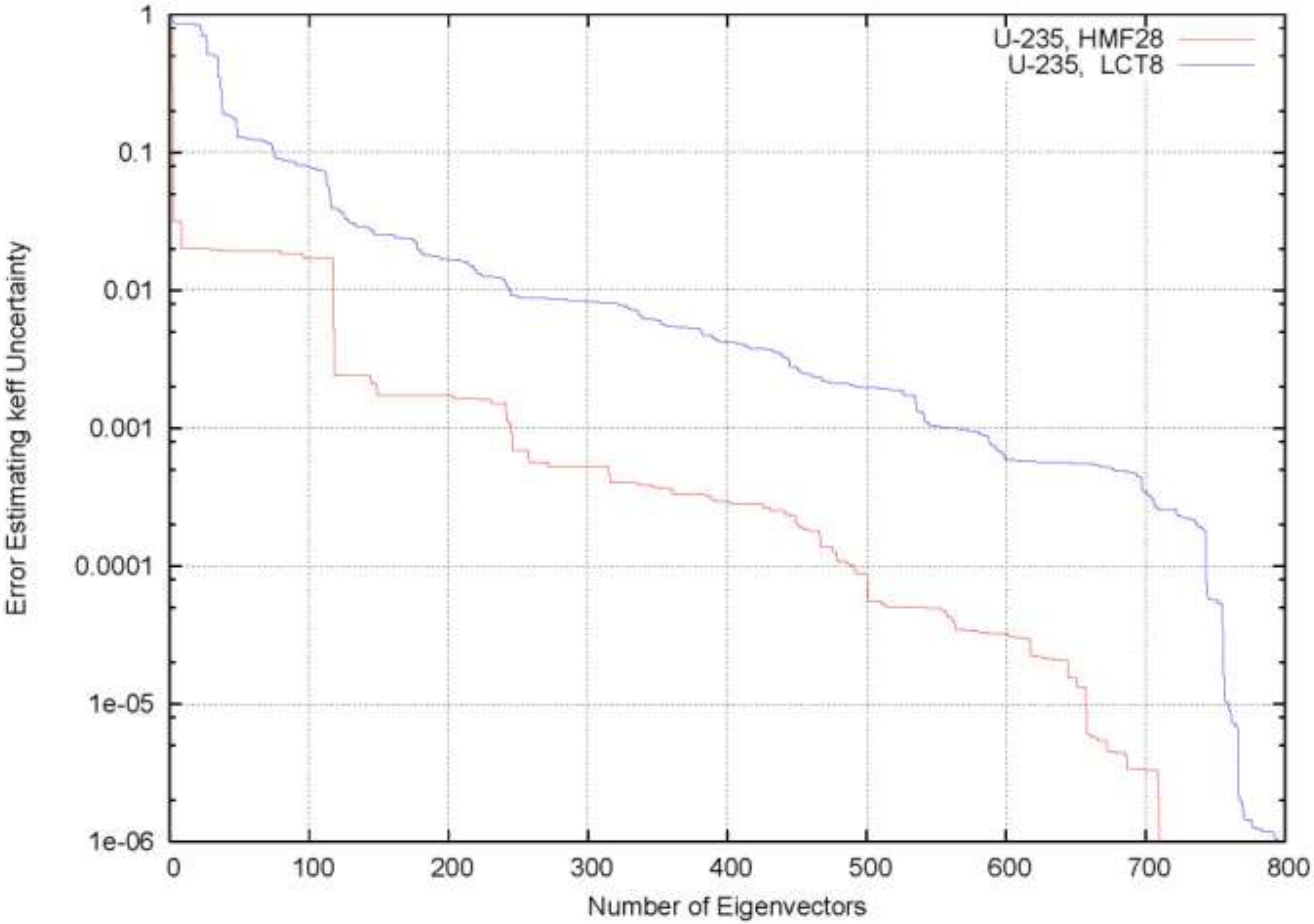

Pu-239, PMF1
Pu-239, PST9
Error Estimating keff Uncertainty
Number of Eigenvectors
1
0.1
0.01
0.001
0.0001
1e-05
1e-06
1e-07
0
50
100
150
200
250
300
350
400

U-235/238

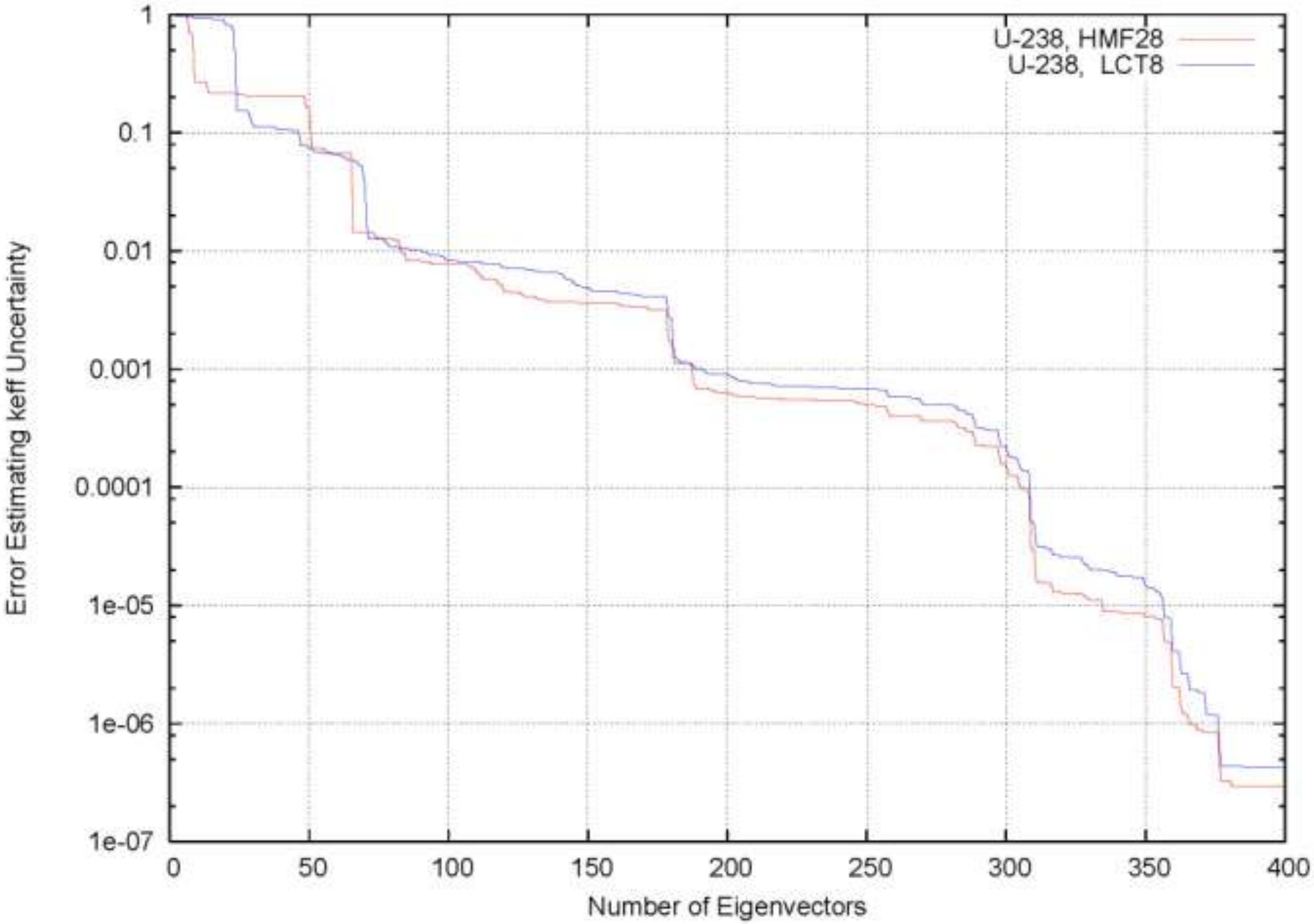
- Covariance data
  - Reactions: total, fission, elastic, inelastic, capture, (n,2n), (n,3n)
  - Energy groups:
    - U-235: 671
    - U-238: 690
  - ERRORR File Size:
    - 39 MB
    - 43 MB
- Benchmarks
  - Flattop-HEU (HEU-MET-FAST-026)
  - LEU Lattice (LEU-COMP-THERM-008)
- Maximum error *E* versus percent memory savings *S*:

E	10^{-2}	10^{-3}	10^{-4}	10^{-5}
S (U-235)	84%	62%	51%	49%
S (U-238)	93%	87%	80%	74%

U-235


U-235, HMF28
U-235, LCT8
Error Estimating keff Uncertainty
1
0.1
0.01
0.001
0.0001
1e-05
1e-06
0
100
200
300
400
500
600
700
800
Number of Eigenvectors

U-238


U-238, HMF28
U-238, LCT8
Error Estimating keff Uncertainty
1
0.1
0.01
0.001
0.0001
1e-05
1e-06
1e-07
0
50
100
150
200
250
300
350
400
Number of Eigenvectors

Relation to the Residual

- **For a fixed residual *R*, find the maximum error *E* for the benchmarks:**

R	Pu-239	U-235	U-238
10^{-3}	1.3×10^{-2}	8.9×10^{-3}	1.1×10^{-2}
10^{-4}	8.6×10^{-4}	1.1×10^{-3}	9.0×10^{-4}
10^{-5}	7.5×10^{-7}	3.2×10^{-4}	3.4×10^{-7}

- **Memory reduction for *R* = 1×10^{-4}:**
  - **Pu-239 72%**
  - **U-235 65%**
  - **U-238 86%**

- **Comment: Fission nu and chi tend to be even more compressible and therefore expected savings may be greater still.**

Summary & Future Work

Summary

- **Modification to ACE proposed for covariance data using principal eigenvectors.**

- **Results suggest that significant memory savings possible while providing accurate assessments of uncertainty in keff.**

- **Need more isotopes, more benchmarks, and different responses to find acceptable residual value(s) for compression.**

Questions?