Similarity Assessment with TSUNAMI

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Introduction to SCALE Methodologies
SCALE Users' Group Workshop
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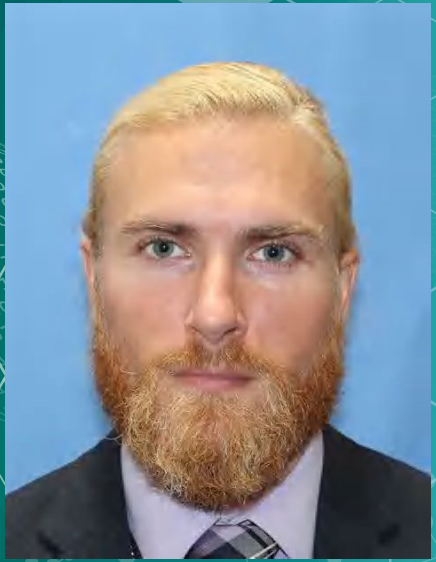


Outline

- BRIEF intro to sensitivity coefficients
- "Fundamental theorem of TSUNAMI"
- Uncertainty propagation and correlation coefficients
- Similarity assessment via integral index c_k
- Conclusion

Introduction to Sensitivity Coefficients

- Predict the expected change in a response (k) due to a change in some input parameter (Σ)
  - These responses can be k_{eff} (or ratios of reaction rates)
  - These input parameters are typically nuclear data
    - Cross sections, multiplicity (nubar: $\bar{\nu}$), fission spectrum (chi: χ)
- The coefficients are dimensionless ratios
  - What would happen to the system k_{eff} if some piece of data were changed by some amount?
  - The coefficient is calculated *without* making the change

$$S_{k,\Sigma} = \frac{\delta k / k}{\delta \Sigma / \Sigma}$$

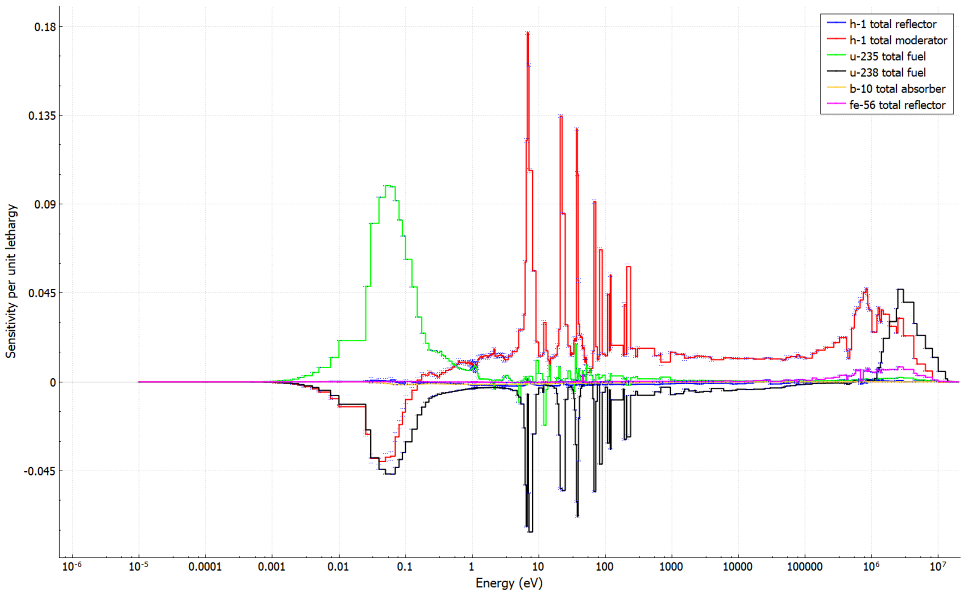
TSUNAMI Sensitivity Methods

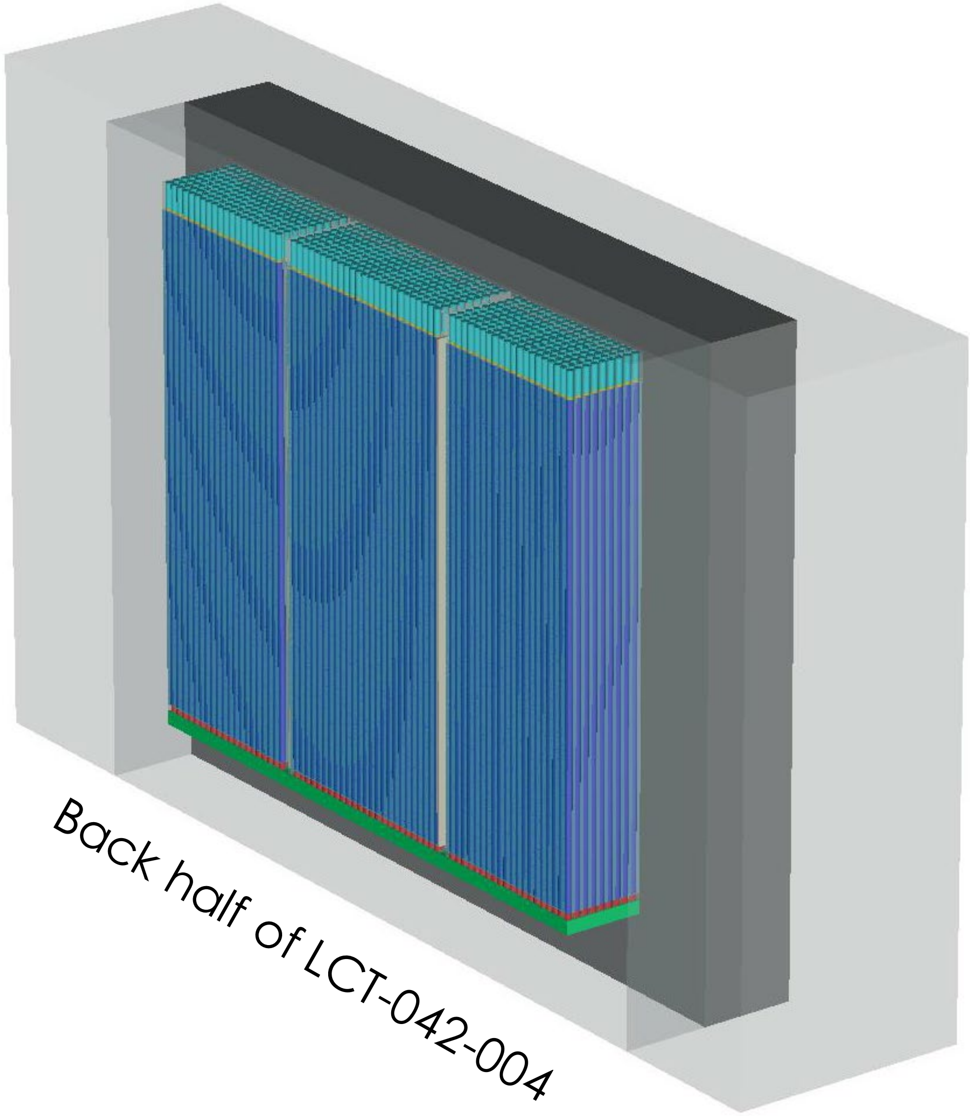
1. **TSUNAMI-1D**
   Deterministic, Multigroup
2. **TSUNAMI-2D**
   Deterministic, Multigroup
3. **TSUNAMI-3D**
   - **Multigroup TSUNAMI-3D**
     Monte Carlo, Multigroup
   - **Iterated Fission Probability (IFP) Method**
     Monte Carlo, Continuous-Energy
   - **CLUTCH Method**
     Monte Carlo, Continuous-Energy

- TSUNAMI offers several options for sensitivity calculations based on the transport code used for analysis. The accuracy and runtime of the approaches vary.

Sensitivities of k_{eff} for a Critical Experiment

Nuclide	Material	Sensitivity	Unc.
H-1	Moderator	0.2396	0.6%
U-235	Fuel	0.2415	0.1%
U-238	Fuel	-0.1395	0.1%
B-10	Absorber	-0.0097	0.2%
Fe-56	Reflector	0.0199	0.5%





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Use of uncertainty information to assess system similarity

- “Fundamental theorem of TSUNAMI”: bias is caused by errors in cross section data, which are bounded by cross-section uncertainties
- Systems will have similar computational biases if they have similar sensitivities
  - Uncertainties act like a weighting function
- Comparison must examine nuclide-, reaction-, and energy-dependent data

Code validation with TSUNAMI

- Some questions TSUNAMI analysis is intended to answer:
  - Which experiments should I use to validate my application?
  - Is there a quantitative basis for generating a reactivity allowance for a validation weakness or gap?
  - Is there a basis for extracting relevant information from existing experiments to largely dissimilar applications?
- TSUNAMI-IP performs
  - Uncertainty analysis
  - Benchmark experiment selection (Similarity assessment)

Propagation of Cross Section Uncertainties

- Chain rule allows for propagation of cross section uncertainty (i.e. covariance) to quantify the data-induced uncertainty in k_{eff} (σ_k^2)

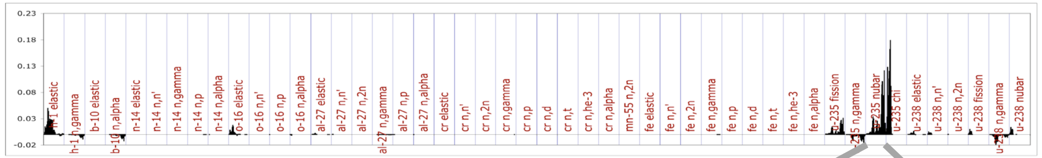
$$\sigma_k^2 = S\ C_{\alpha\alpha} S^T$$

Where:

- S is a matrix of all energy-dependent sensitivity data for all systems considered (S^T is transpose)
- $C_{\alpha\alpha}$ is a matrix containing energy-dependent covariance information evaluated for all nuclear data

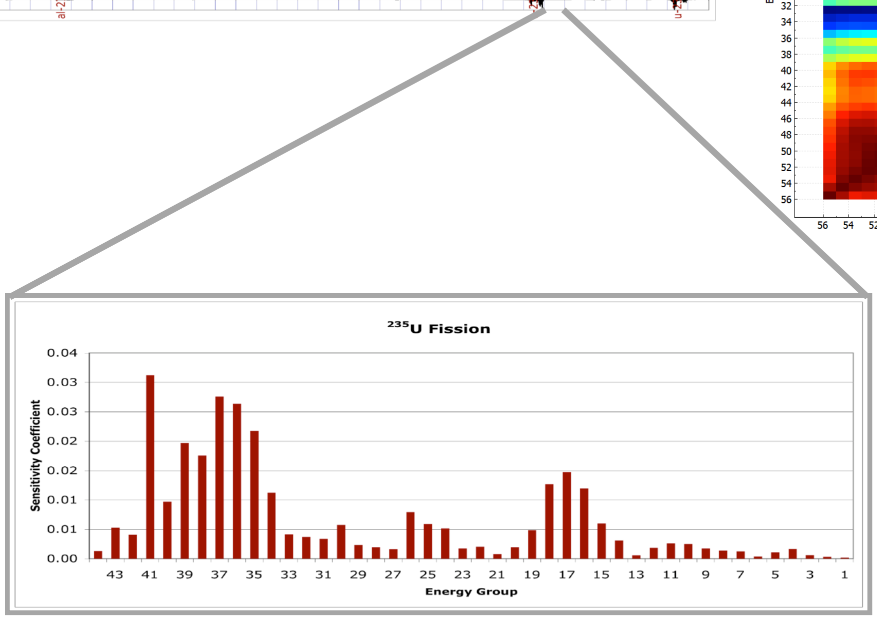
Uncertainty Propagation

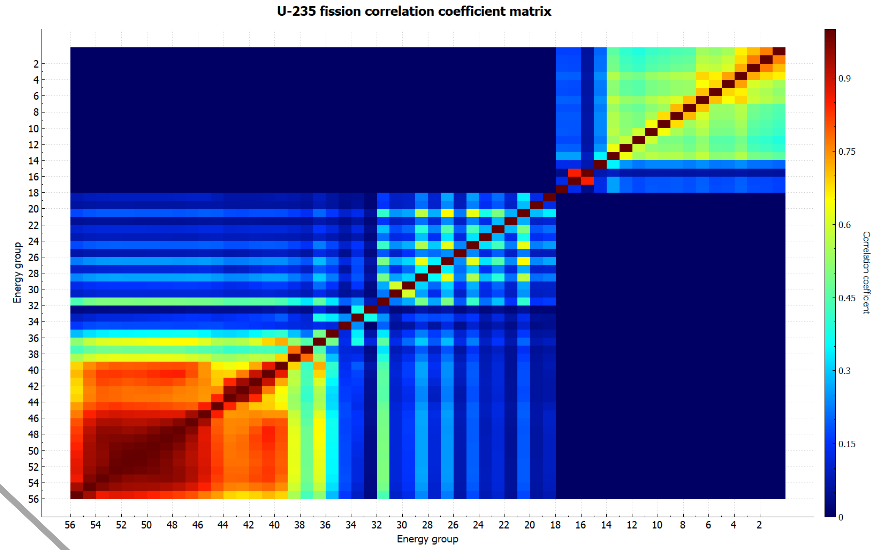
- Uncertainty in k_{eff} of a single system



S

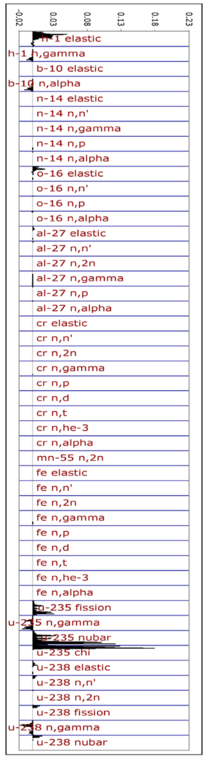
$$\frac{dk/k}{d\Sigma/\Sigma}$$





$C_{\alpha\alpha}$

$$\left(\frac{\Delta\Sigma}{\Sigma}\right)^2$$



S^T

$$\frac{dk/k}{d\Sigma/\Sigma}$$

$$= \sigma^2$$

C_{kk}

$$\left(\frac{\Delta k}{k}\right)^2$$

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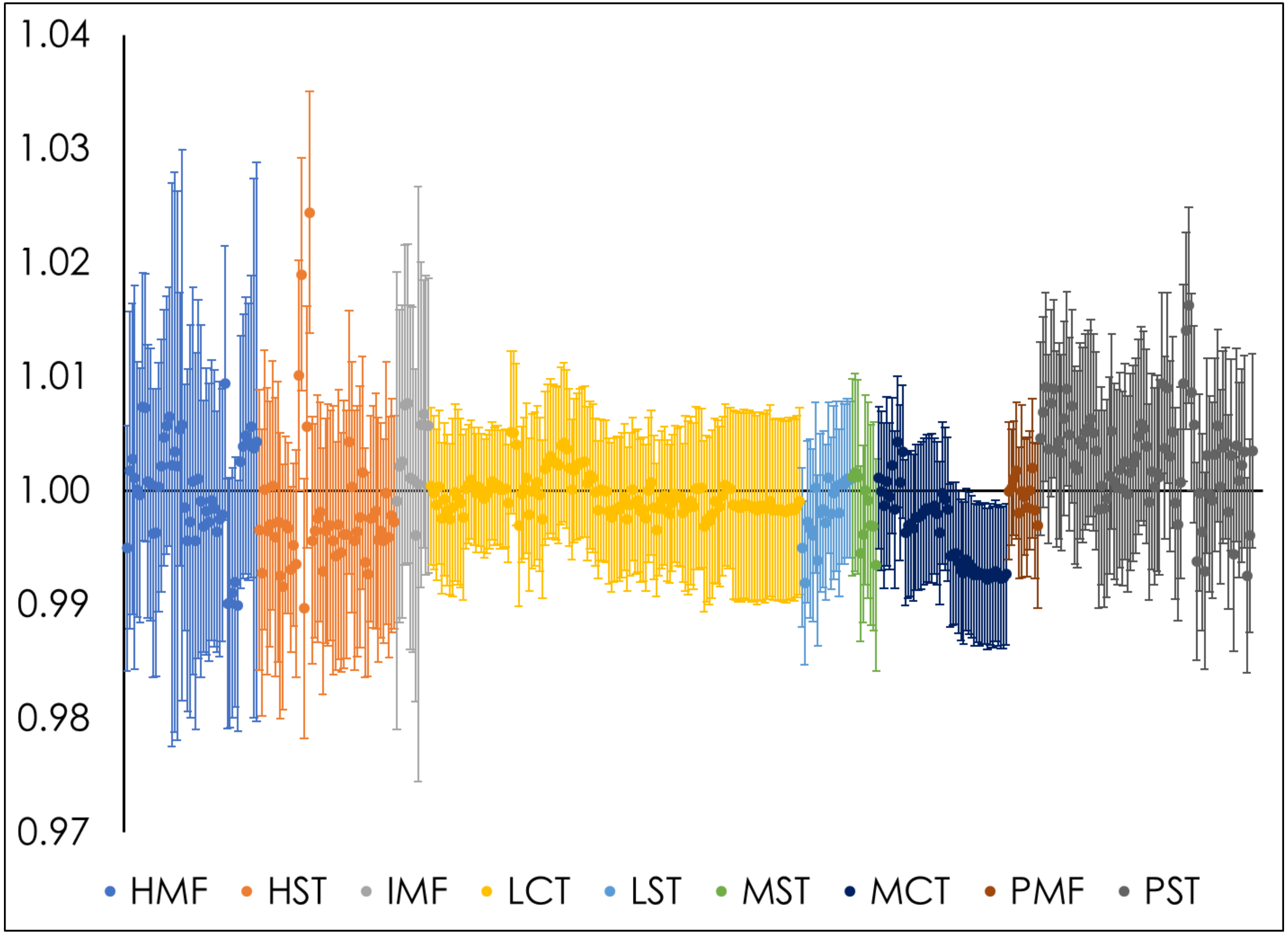
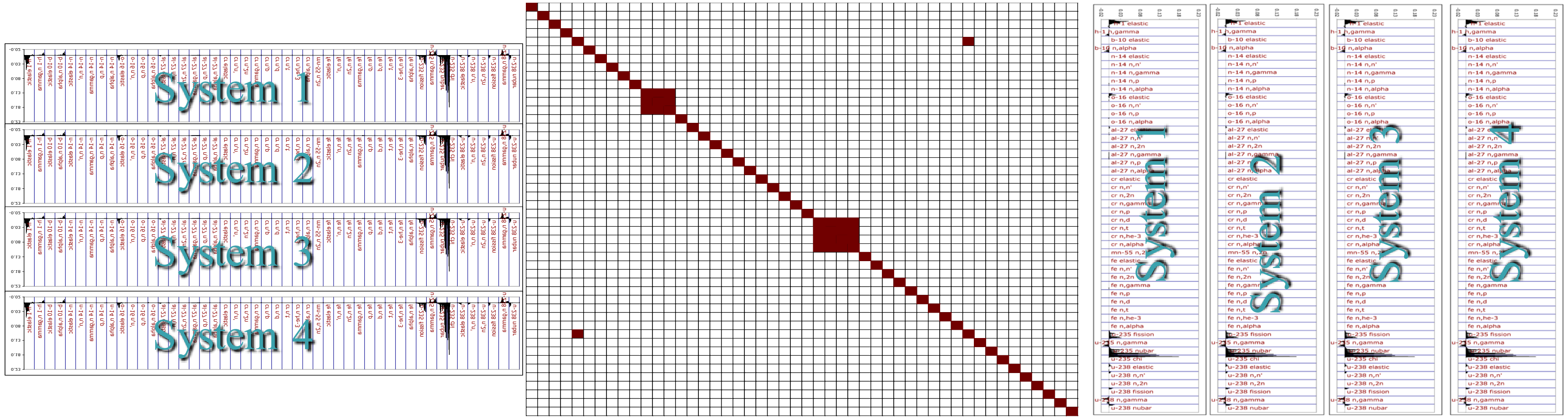
Uncertainties for Criticality Benchmarks

- Results from SCALE 6.2.2 Validation Report
- ~96.5% of C/E values within 1σ of unity



Uncertainty Propagation

- Suppose we have sensitivity information for multiple systems:



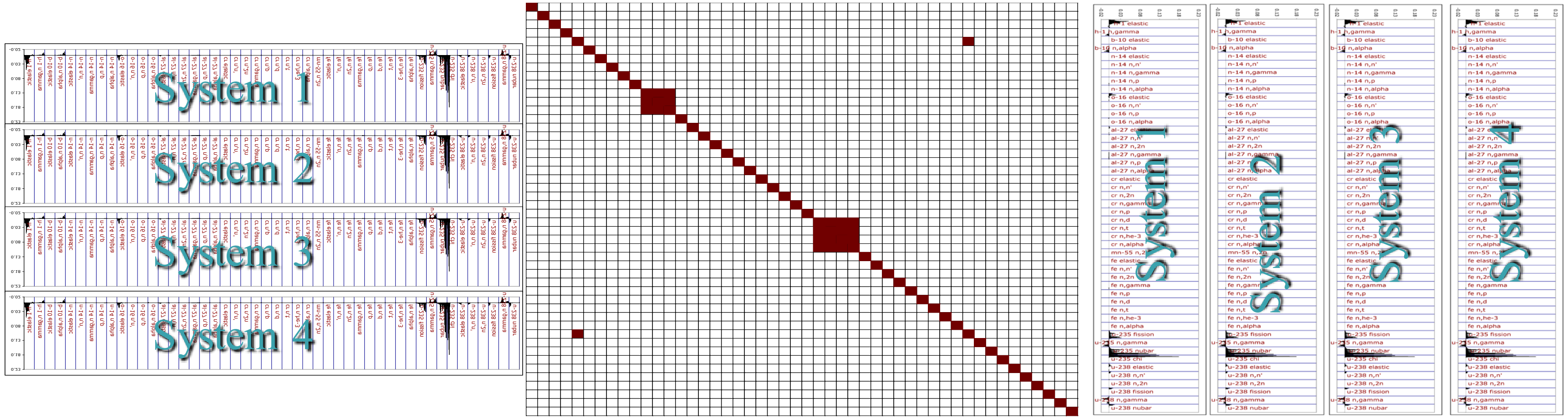
S $\qquad$ $C_{\alpha\alpha}$ $\qquad$ S^T

Diagonal elements are variance in each system

$$= \begin{bmatrix} \sigma_{11}^2 & & & \\ & \sigma_{22}^2 & & \\ & & \sigma_{33}^2 & \\ & & & \sigma_{44}^2 \end{bmatrix}$$

Uncertainty Propagation

- Suppose we have sensitivity information for multiple systems:



S $C_{\alpha\alpha}$ S^T

$$= \begin{bmatrix} & \sigma_{12}^2 & \sigma_{13}^2 & \sigma_{14}^2 \\ \sigma_{21}^2 & & \sigma_{23}^2 & \sigma_{24}^2 \\ \sigma_{31}^2 & \sigma_{32}^2 & & \sigma_{34}^2 \\ \sigma_{41}^2 & \sigma_{42}^2 & \sigma_{43}^2 & \end{bmatrix}$$

Off-diagonal elements are covariance between two systems

Correlation Coefficient c_k for System 1 and System 4

$$c_{kk} = \begin{vmatrix} \sigma_{11}^2 & \sigma_{12}^2 & \sigma_{13}^2 & \sigma_{14}^2 \\ \sigma_{21}^2 & \sigma_{22}^2 & \sigma_{23}^2 & \sigma_{24}^2 \\ \sigma_{31}^2 & \sigma_{32}^2 & \sigma_{33}^2 & \sigma_{34}^2 \\ \sigma_{41}^2 & \sigma_{42}^2 & \sigma_{43}^2 & \sigma_{44}^2 \end{vmatrix}$$

$$c_k = \frac{\sigma_{41}^2}{\sqrt{\sigma_{11}^2}\sqrt{\sigma_{44}^2}}$$

Integral Index c_k

- c_k is an integral index used to assess similarity
  - Uncertainty weighted sensitivity profiles between two systems
    - Typically an application system and a critical experiment
  - What fraction of the data-induced uncertainty is shared by two systems?
  - Correlation coefficient, so normalized from -1.0 to +1.0
    - +1.0 is exactly the same system while 0 is completely uncorrelated
- Current guidance:
  - c_k of 0.9 or higher indicates a highly similar system
  - c_k between 0.8 and 0.9 are "marginally" similar

c_k calculation

- c_k calculated by TSUNAMI-IP
- Each application compared with each experiment

Integral Indices for All Experiments in Relation to All Applications

Values colored Blue exceed cutoff value

Values colored Red are maximum for each application

Application #1
gbc-32 - buc w17x17, 1.0 - 6

NUMBER	EXPERIMENT	Type	Format	Value	Xsec Uncert	c_k ↑
111	lct049, case 18, maracas, h/	keff	Relative	1.0015E+0 ± 4.9700E-4	5.53031E-1 ± 4.2903E-5 % dk/k	0.7455 ± 0.0009
97	lct049, case 4, maracas, h/u	keff	Relative	9.9928E-1 ± 4.9700E-4	5.72524E-1 ± 5.7411E-5 % dk/k	0.7363 ± 0.0008
96	lct049, case 3, maracas, h/u	keff	Relative	9.9866E-1 ± 4.2700E-4	5.74281E-1 ± 5.0922E-5 % dk/k	0.7354 ± 0.0008
94	lct049, case1, maracas, h/u=	keff	Relative	9.9783E-1 ± 4.9900E-4	5.78241E-1 ± 5.5989E-5 % dk/k	0.7328 ± 0.0009
95	lct049, case 2, maracas, h/u	keff	Relative	9.9943E-1 ± 4.9600E-4	5.82083E-1 ± 6.5012E-5 % dk/k	0.7314 ± 0.0009
101	lct049, case 8, maracas, h/u	keff	Relative	9.9771E-1 ± 4.9800E-4	5.93696E-1 ± 6.1676E-5 % dk/k	0.7246 ± 0.0011
110	lct049, case 17, maracas, h/	keff	Relative	9.9902E-1 ± 4.9000E-4	5.94144E-1 ± 5.6457E-5 % dk/k	0.7237 ± 0.0011
148	mix-comp-therm-004-003	keff	Relative	9.9677E-1 ± 2.5800E-4	6.34278E-1 ± 1.6177E-4 % dk/k	0.7182 ± 0.0009

- Extended c_k edit from TSUNAMI-IP
- Contribution of each covariance matrix location (largely isotope-reaction) to c_k

Application #1
gbc-32 - buc w17x17, 1.0 - 6 with
Experiment #111
lct049, case 18, maracas, h/

The c_k value is: 0.7455 ± 0.0009

Contributions to c_k by individual energy covariance matrices:

The c_k value is the sum of the individual contributions.

Input covariance file: 56groupcov7.1

Working covariance file: tsunami-ip_sample.wrk

Covariance Matrix		c_k Contribution	Individual c_k
Nuclide-Reaction	Nuclide-Reaction	Due to this Matrix	From this Matrix
^{235}U nubar	^{235}U nubar	2.7967E-01 ± 8.8787E-06	9.9977E-01 ± 3.1739E-05
^{238}U n,gamma	^{238}U n,gamma	2.3888E-01 ± 4.2904E-05	9.8109E-01 ± 1.7621E-04
^{235}U n,gamma	^{235}U n,gamma	6.5028E-02 ± 1.2896E-05	9.4240E-01 ± 1.8689E-04
^{238}U n,n'	^{238}U n,n'	6.2786E-02 ± 8.4151E-04	9.9993E-01 ± 1.3402E-02
^{238}U nubar	^{238}U nubar	2.5906E-02 ± 2.3041E-06	9.9993E-01 ± 8.8932E-05
^{235}U fission	^{235}U fission	2.3404E-02 ± 6.9609E-06	9.7662E-01 ± 2.9047E-04
^{235}U fission	^{235}U n,gamma	2.0116E-02 ± 6.5511E-06	
^{1}H elastic	^{1}H elastic	1.4180E-02 ± 4.4734E-05	9.9896E-01 ± 3.1513E-03
^{238}U elastic	^{238}U n,n'	-1.4143E-02 ± 1.2650E-04	
^{235}U n,gamma	^{235}U fission	1.0555E-02 ± 2.1524E-06	

Summary

- S/U-based parameters should be useful in identifying similar benchmark systems
  - Basis for similarity is both sensitivity information and nuclear data uncertainties
  - Use of c_k has been integrated into other validation approaches
- Similarity assessment can be used in trending analyses to determine subcritical limits
- ORNL recommends c_k values greater than 0.8 for inclusion in validation