

TSUNAMI-IP tool for similarity assessment

SCALE 6.3.2

ORNL is managed by UT-Battelle, LLC for the US Department of Energy

Learning goals

- **Gain familiarity** with the key concepts of propagation of cross section uncertainties and similarity assessment
- **Demonstrate** the use of TSUNAMI-IP for uncertainty propagation and similarity assessment

Role of TSUNAMI-IP within the TSUNAMI suite

- The TSUNAMI suite implements the SCALE sensitivity/uncertainty (S/U) analysis methods
- TSUNAMI-IP performs both uncertainty analysis and similarity assessment, enabling benchmark experiment selection
- 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 any appropriate basis for extrapolating information from existing experiments to applications for which no similar experiments exist?

See <https://scale-manual.ornl.gov/tsunami-ip.html>

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)

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

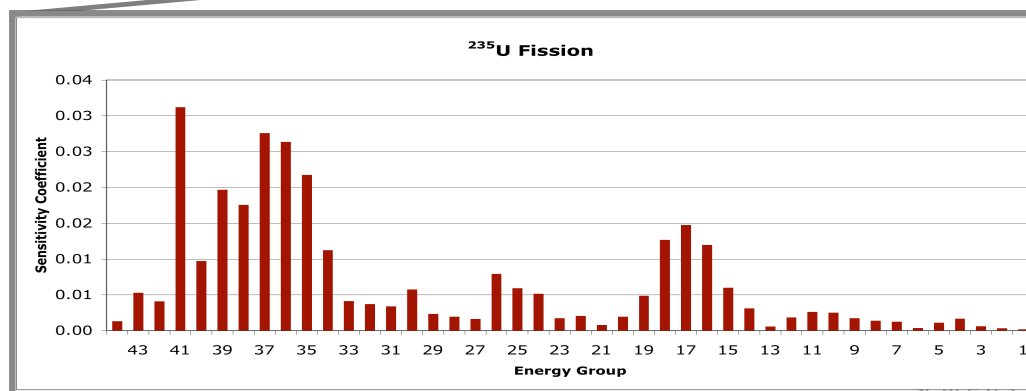
Where:

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

Propagation of cross section uncertainties

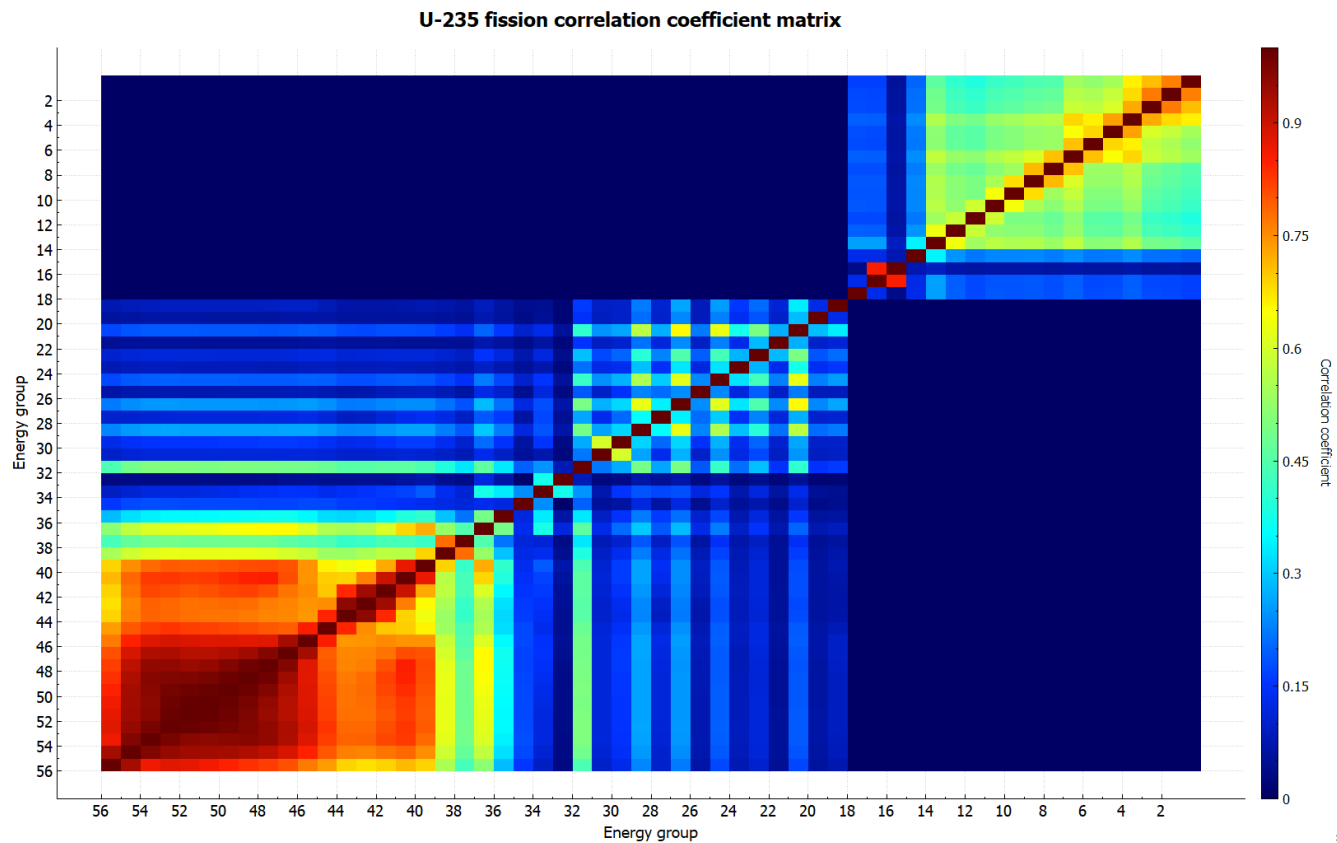
- Matrix of sensitivity coefficients
 - For each nuclide in the problem, the sensitivity to each reaction is stored in energy-dependent bins. For example:

h-1 elastic
 h-1 n, gamma
 b-10 elastic
 b-10 n, alpha
 n-14 elastic
 n-14 n, gamma
 n-14 n, p
 n-14 n, alpha
 o-16 elastic
 o-16 n, n'
 o-16 n, alpha
 al-27 elastic
 al-27 n, n'
 al-27 n, 2n
 al-27 n,
 gamma
 al-27 n, p
 cr elastic
 cr n, n'
 cr n, 2n
 cr n, gamma
 cr n, p
 cr n, d
 cr n, t
 cr n, he-3
 cr n, alpha
 mn-55 n, 2n
 fe elastic
 fe n, 2n
 fe n, gamma
 fe n, p
 fe n, t
 fe n, he-3
 fe n, alpha
 u-235 fission
 u-235 n,
 gamma
 u-235 nubar
 u-235 chi
 u-238 elastic
 u-238 n, n'
 u-238 n, 2n
 u-238 fission
 u-238 n,
 gamma
 u-238 nubar



Propagation of cross section uncertainties

- $C_{\alpha\alpha}$ Covariance Matrix



- Uncertainty in k_{eff} of a single system: Combine the pieces via the “sandwich formula”



$C_{\alpha\alpha}$

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



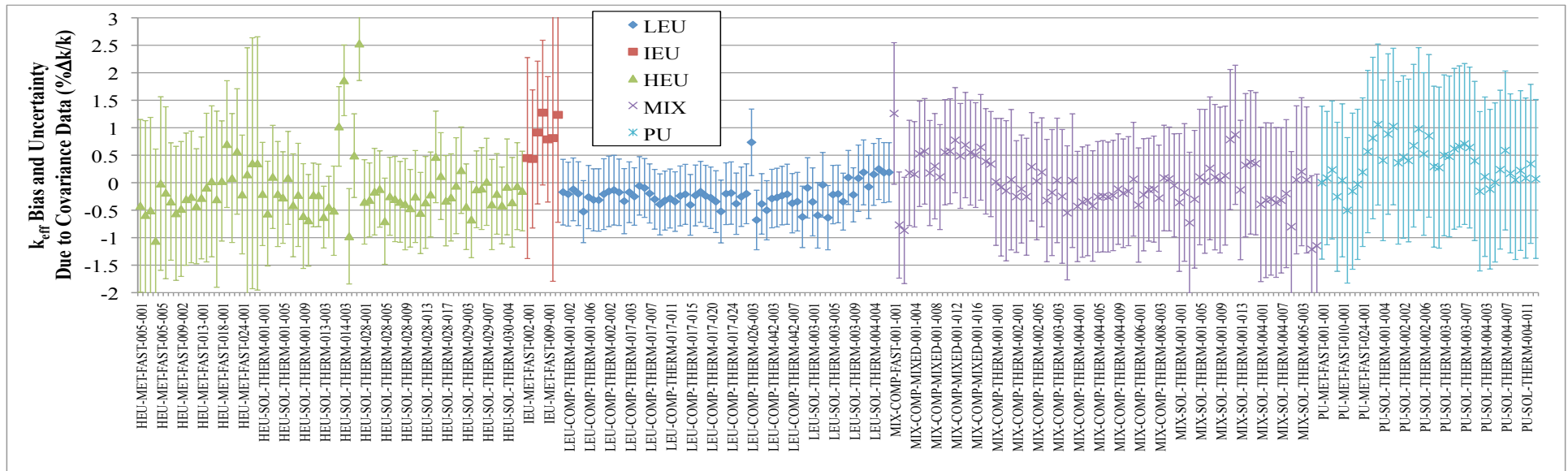
$$\frac{dk/k}{d\Sigma/\Sigma}$$



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

Example of propagated uncertainties for criticality benchmarks

For a selection of ICSBEP benchmarks, the plot below shows the k_{eff} bias (C – E) **with** associated uncertainty propagated from nuclear data covariances (the error bars in the figure).



"Skeleton" TSUNAMI-IP input

```
=tsunami-ip
title-goes-here
read parameters
' TSUNAMI-IP analysis parameters:
  "turn on/off" c, uncertainty, other calculations
end parameters
read applications
' path to application SDF(s)
end applications
read experiments
' path to experiment SDF(s)
end experiments
read response
' Optional alternative to application/experiment blocks
end response
read covariance
' Optional: detailed control for covariance "patching"
end covariance
read reactions
' Optional: specify nuclide-reaction pairs for, e.g.,
' analysis via the g similarity index
end reactions
read exclusions
' Optional: specify reactions to exclude from
' cr index analyses
end exclusions
read html
' Optional: Customize HTML output
end html
end
```

Notes:

- To activate the calculation of k_{eff} uncertainties such as those shown on the previous slide, add the keyword *uncert* to the **parameters** block.
- The sensitivity data are provided via Sensitivity Data Format (SDF) files, as computed by a TSUNAMI calculation
- The covariance data can be selected via the *coverx=[file]* in the **parameters** block. The default covariance file is the 56groupcov7.1 that is included with the SCALE data.
 - Analyses may encounter the need to augment the available covariance data. This can be done with "fine tuning" with the **covariance** block, or with a variety of default options provided via the **parameters** block.

TSUNAMI-IP output: Uncertainty in k_{eff}

Application #1 gbc-32 - buc w17x17, 1.0 - 6					
NUMBER	EXPERIMENT	Type	Format	Value	Xsec Uncert
1	heu-met-fast-005a	keff	Relative	9.9581E-1 ± 4.9200E-4	1.49128E+0 ± 1.5356E-4 % dk/k
2	heu-met-fast-005b	keff	Relative	9.9482E-1 ± 4.9900E-4	1.71537E+0 ± 1.6844E-4 % dk/k
3	heu-met-fast-005c	keff	Relative	9.9456E-1 ± 5.0000E-4	1.69785E+0 ± 2.0329E-4 % dk/k
4	heu-met-fast-005d	keff	Relative	9.8832E-1 ± 4.9700E-4	1.67351E+0 ± 1.7224E-4 % dk/k
5	heu-met-fast-005e	keff	Relative	9.9785E-1 ± 4.8900E-4	1.58395E+0 ± 1.5879E-4 % dk/k
6	heu-met-fast-005f	keff	Relative	9.9688E-1 ± 4.9900E-4	1.54034E+0 ± 1.6757E-4 % dk/k
7	heu-met-fast-008-001	keff	Relative	9.9547E-1 ± 1.0000E-4	1.10478E+0 ± 5.3334E-4 % dk/k
8	heu-met-fast-009-001	keff	Relative	9.9364E-1 ± 1.0000E-4	1.25586E+0 ± 5.2098E-4 % dk/k
9	heu-met-fast-009-002	keff	Relative	9.9443E-1 ± 1.0000E-4	1.22716E+0 ± 6.0693E-4 % dk/k
10	heu-met-fast-010-001	keff	Relative	9.9620E-1 ± 1.0000E-4	1.23428E+0 ± 5.9228E-4 % dk/k
11	heu-met-fast-010-002	keff	Relative	9.9661E-1 ± 1.0000E-4	1.21514E+0 ± 5.9023E-4 % dk/k

- Request computation of uncertainty with parameter input *uncert*
- Request table of values with parameter input *values*

TSUNAMI-IP output: Extended uncertainty edit

Application #1 gbc-32 - buc w17x17, 1.0 - 6		
the standard deviation of keff (% dk/k) is: 4.197E-01 ± 1.453E-04 percent		
contributions to uncertainty in keff (% dk/k) by individual energy covariance matrices:		
Covariance Matrix		Unc. in % dk/k
Nuclide-Reaction	Nuclide-Reaction	Due to this Matrix
²³⁵ U nubar	²³⁵ U nubar	1.9967E-01 ± 3.7053E-06
²³⁸ U n,gamma	²³⁸ U n,gamma	1.9335E-01 ± 1.4395E-05
²³⁹ Pu fission	²³⁹ Pu fission	1.4652E-01 ± 1.2739E-05
²³⁹ Pu fission	²³⁹ Pu n,gamma	1.1244E-01 ± 6.0440E-06
²³⁹ Pu n,gamma	²³⁹ Pu n,gamma	9.7689E-02 ± 6.6390E-06
²³⁵ U n,gamma	²³⁵ U n,gamma	8.3645E-02 ± 4.2012E-06
¹ H n,gamma	¹ H n,gamma	7.7437E-02 ± 3.0568E-06
²³⁵ U fission	²³⁵ U fission	7.2681E-02 ± 4.6763E-06

- Request extended uncertainty (nuclide-reaction data) with parameter *uncert_long*

Any questions before we move on to similarity assessment?

- We will practice with both similarity assessment and uncertainty analysis later on...



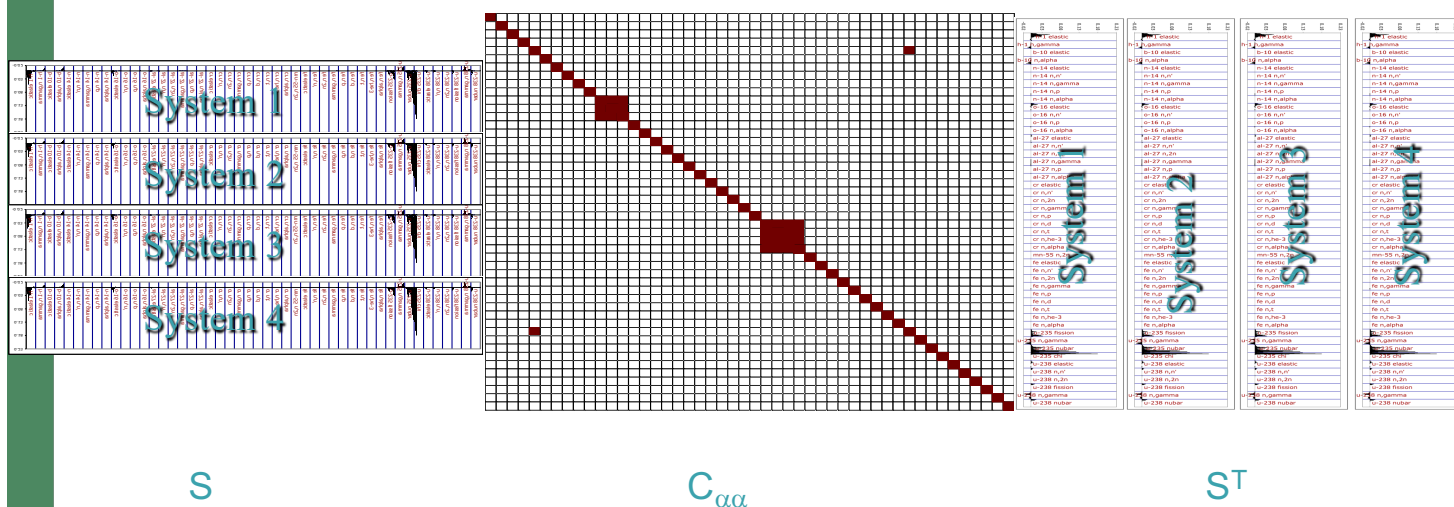
Use of uncertainty information to assess system similarity

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

- Suppose we have sensitivity information for multiple systems:

Uncertainty propagation (cont.)

- Suppose we have sensitivity information for multiple systems:

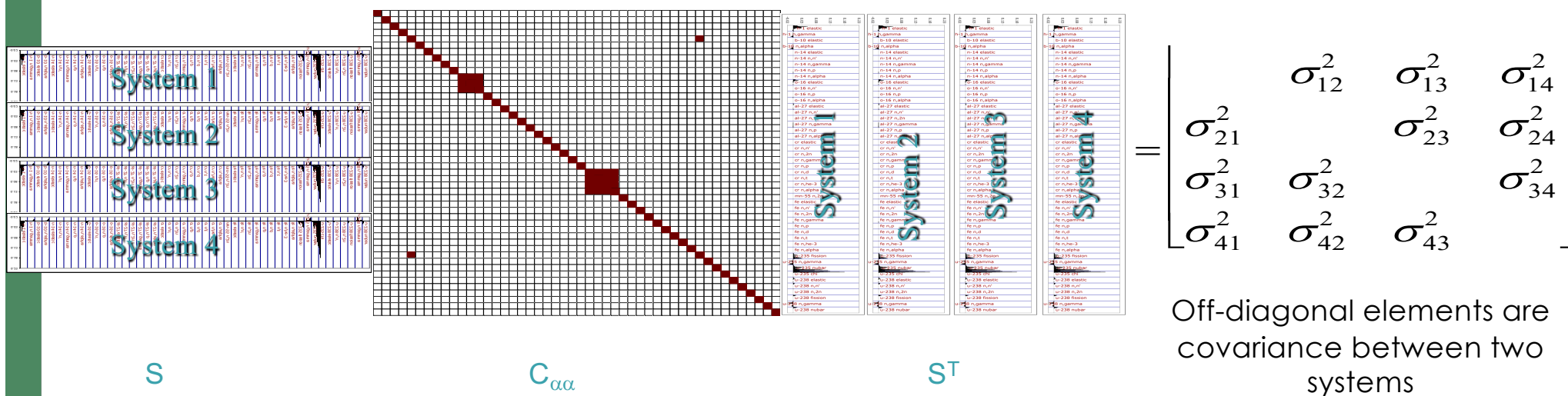


Diagonal elements are variance in each system

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

Uncertainty propagation (cont.)

- Suppose we have sensitivity information for multiple systems:



Correlation coefficient c_k for System 1 and System 4

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

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

Integral index c_k

- c_k is an integral index used to assess similarity
 - Uncertainty weighted sensitivity profiles between a design system and a criticality 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 with TSUNAMI-IP

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	$c_k \uparrow$
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

- To request c_k from TSUNAMI-IP, enter c in parameter input and *values* to generate summary table
- Parameter *cvalue* sets minimum threshold on c_k for summary data, requested with parameter *csummary*

TSUNAMI-IP output: Extended c_k edit

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	$2.7967\text{E-}01 \pm 8.8787\text{E-}06$	$9.9977\text{E-}01 \pm 3.1739\text{E-}05$
^{238}U n_gamma	^{238}U n_gamma	$2.3888\text{E-}01 \pm 4.2904\text{E-}05$	$9.8109\text{E-}01 \pm 1.7621\text{E-}04$
^{235}U n_gamma	^{235}U n_gamma	$6.5028\text{E-}02 \pm 1.2896\text{E-}05$	$9.4240\text{E-}01 \pm 1.8689\text{E-}04$
^{238}U n,n'	^{238}U n,n'	$6.2786\text{E-}02 \pm 8.4151\text{E-}04$	$9.9993\text{E-}01 \pm 1.3402\text{E-}02$
^{238}U nubar	^{238}U nubar	$2.5906\text{E-}02 \pm 2.3041\text{E-}06$	$9.9993\text{E-}01 \pm 8.8932\text{E-}05$
^{235}U fission	^{235}U fission	$2.3404\text{E-}02 \pm 6.9609\text{E-}06$	$9.7662\text{E-}01 \pm 2.9047\text{E-}04$
^{235}U fission	^{235}U n_gamma	$2.0116\text{E-}02 \pm 6.5511\text{E-}06$	
^1H elastic	^1H elastic	$1.4180\text{E-}02 \pm 4.4734\text{E-}05$	$9.9896\text{E-}01 \pm 3.1513\text{E-}03$
^{238}U elastic	^{238}U n,n'	$-1.4143\text{E-}02 \pm 1.2650\text{E-}04$	
^{235}U n_gamma	^{235}U fission	$1.0555\text{E-}02 \pm 2.1524\text{E-}06$	

- Request extended c_k with parameter c_long

Applications and experiments (or response) data blocks

filename use=R name=N type=T (can be in any order)

- Optional keywords:
- *use=appl, expt, or omit*
- *name=identifier in output (max 20 characters)*
- *type=response type (max 8 characters) (keff: default)*

```
read response
```

```
C:\k_crit_a.sdf name=1_exp type=keff
```

```
C:\k_crit_b.sdf name=2_exp type=keff
```

```
C:\k_crit_c.sdf name=3_exp type=keff use=appl
```

```
end response
```

Sample TSUNAMI-IP input

```
=tsunami-ip
read parameter
c csummary values html username
end parameter
read apps mox-1.sdf mox-2.sdf end apps
read exps
mct002-01sen.sdf mct002-02sen.sdf
mct002-03sen.sdf mct002-04sen.sdf
mmf011-01sen.sdf mmf011-02sen.sdf
mmf011-03sen.sdf mmf011-04sen.sdf
nse55t5-01sen.sdf nse55t5-02sen.sdf
nse55t5-03sen.sdf nse55t5-04sen.sdf
pcm001-01sen.sdf pcm001-02sen.sdf
pcm001-03sen.sdf pcm001-04sen.sdf
end exps
end
```

Using SHELL to copy or link files

- SHELL sequence passes commands to the OS – such as linking or copying input SDF files for convenience
- Current directory is SCALE temporary working directory
- Platform-independent commands can be used starting with SCALE 6.2

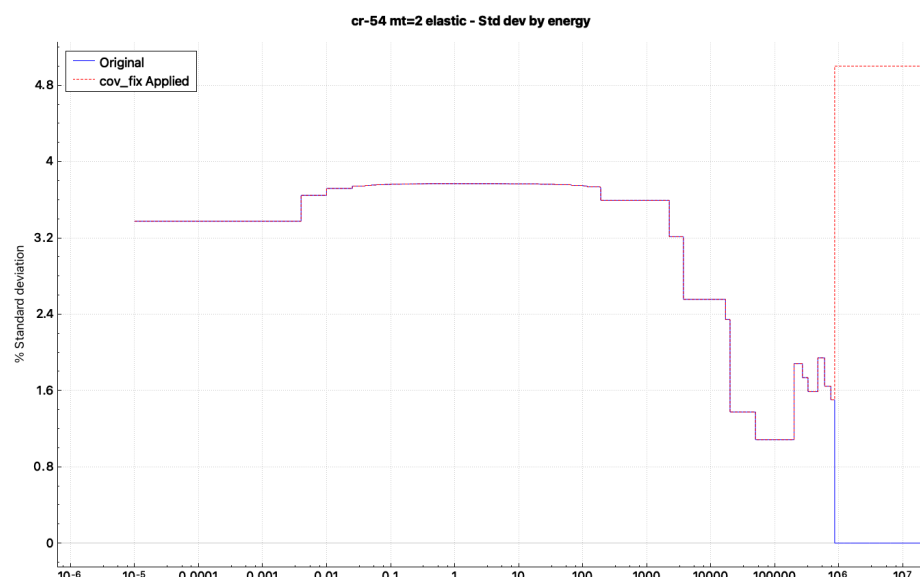
```
=shell
  cp ${INPDIR}/mox-1.sdf ${TMPDIR}
  ln -sf ${INPDIR}/mox-2.sdf ${TMPDIR}
end
=tsunami-ip
read parameter
c csummary values html username
end parameter
read apps mox-1.sdf mox-2.sdf end apps
read exps
mct002-01sen.sdf mct002-02sen.sdf
mct002-03sen.sdf mct002-04sen.sdf
mmf011-01sen.sdf mmf011-02sen.sdf
mmf011-03sen.sdf mmf011-04sen.sdf
nse55t5-01sen.sdf nse55t5-02sen.sdf
nse55t5-03sen.sdf nse55t5-04sen.sdf
pcm001-01sen.sdf pcm001-02sen.sdf
pcm001-03sen.sdf pcm001-04sen.sdf
end exps
end
```

Patching covariance data...

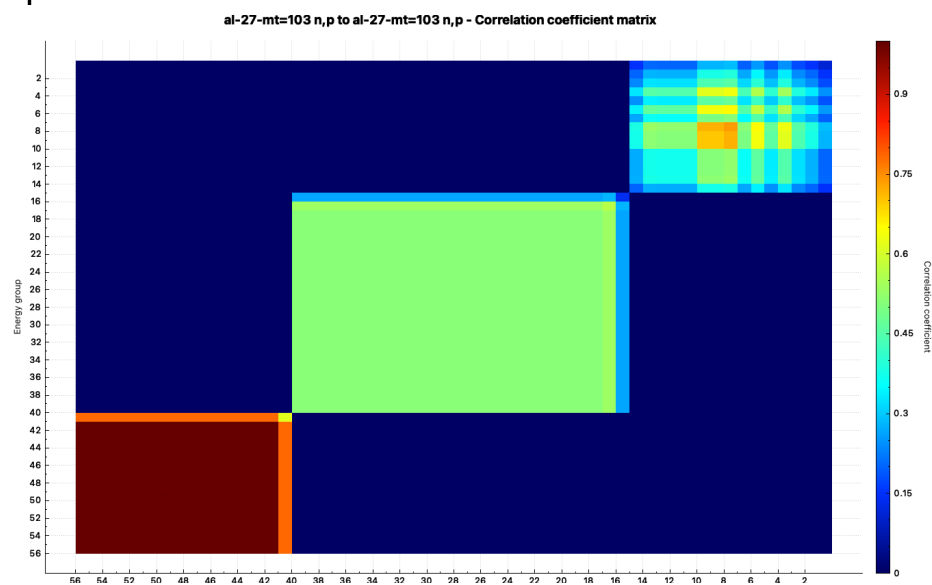
- The covariance library is not exhaustive – some reactions in at least some energy groups for at least some nuclides have no data
 - Other data (like uncertainties greater than 100%) are viewed as junk
- TSUNAMI-IP allows these data to be patched
 - *cov_fix*: Replace zero and large (standard deviation >1000%) values on diagonal of cross-section covariance data with user input values and default values.
 - *use_dcov*: Use user-defined default covariance data for nuclide reaction pairs not included on the covariance data file.
- There are scenarios in which this can have a significant impact
 - Fortunately, water-moderated pin arrays don't tend to be one of them

Patching covariance data...

`cov_fix`: Fixes the range with zero standard deviation to default value



`use_dcov`: Inserts default covariance for nuclide-reaction pairs that have no covariance data



Patching covariance data... (cont.)

- Parameters *udcov_fast*, *udcov_inter*, and *udcov_therm* specify default standard deviation in respective energy ranges when finer control is needed
 - Fully correlated within respective energy ranges
 - Historically values of 40%, 10% or 20%, and 5% have been used
- Any values calculated in an extended c_k or uncertainty edit are flagged if patched data are used

al-27 n,p	al-27 n,p	1.0381E-04 +/- 8.0750E-11 *
cr-54 elastic	cr-54 elastic	9.1691E-05 +/- 1.3890E-10 ***

- Straightforward to turn on and off and gauge impact

Summary

- S/U-based parameters can be useful in identifying similar benchmark systems
 - Basis for similarity is both sensitivity information and nuclear data uncertainties
- Similarity assessment can be used in trending analyses to determine subcritical limits
- Uncertainty analysis can be used to support determination of margins for validation gaps and weaknesses
- ORNL recommends c_k values greater than 0.8 for inclusion in validation

See <https://scale-manual.ornl.gov/tsunami-ip.html>

Questions?