Impact of Correlated Benchmark Experiments on the Computational Bias in Criticality Safety Assessment

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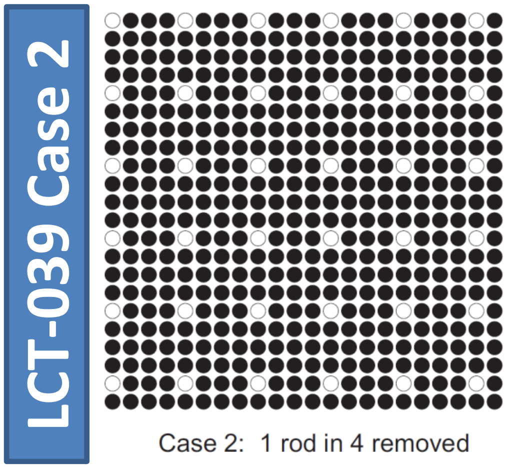
Introduction

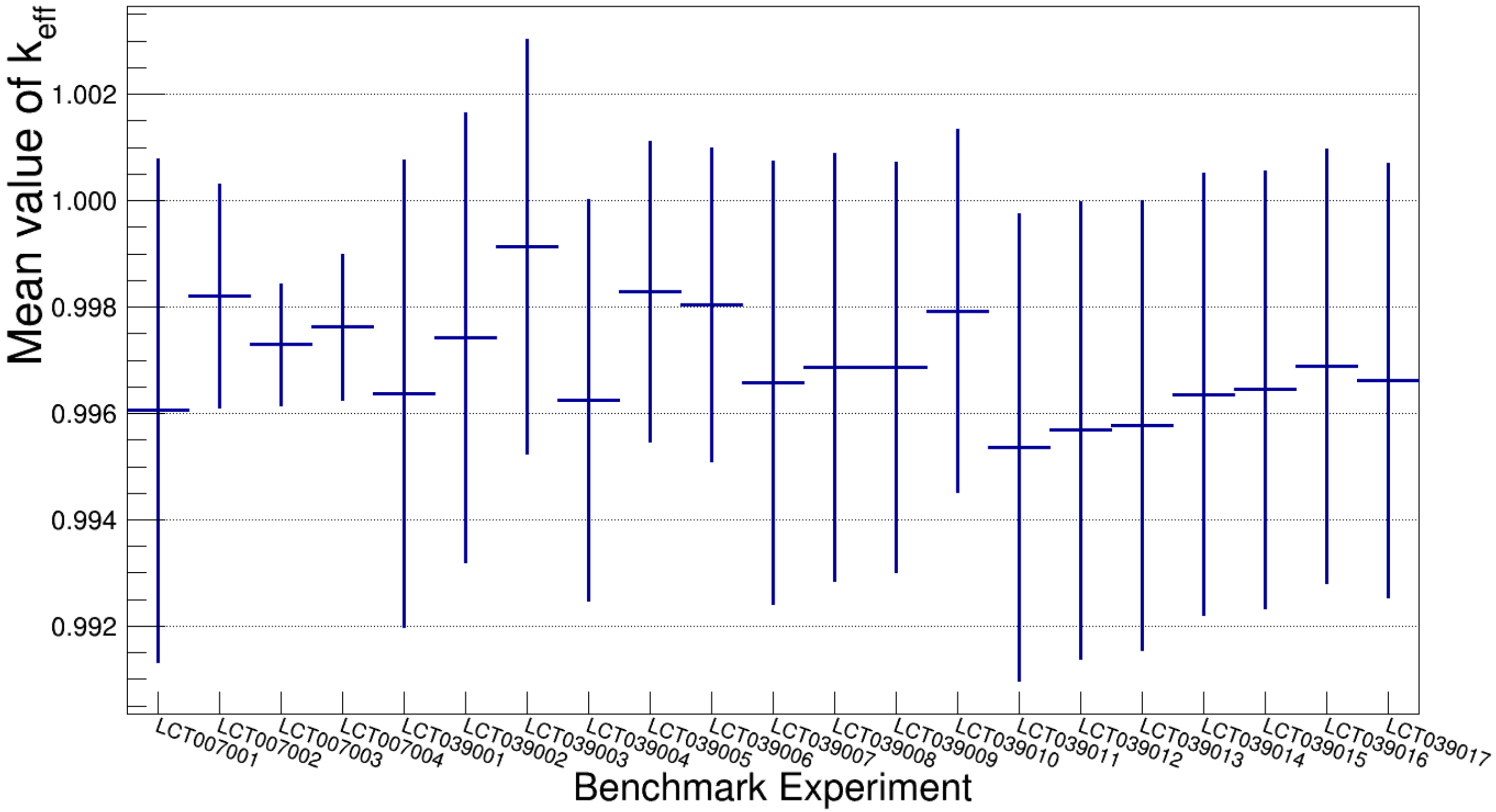
- Code validation is an important issue in criticality safety assessments
- Typically critical experiments are performed in series using the same apparatus and experimental equipment
- Determine the impact of correlated benchmark experiments on the computational bias
- Based on a benchmark proposal discussed at the 2012 meeting of the UACSA Expert Group of the OECD/NEA, Uncertainty analysis was used to derive the correlation matrix between the k_{eff} values of 21 cases of the experiment LCT-007 and LCT-039
- So far, two methods are used to derive the computational bias:
  - Trending analysis
  - TSUNAMI/TSURFER



Case 2: 1 rod in 4 removed

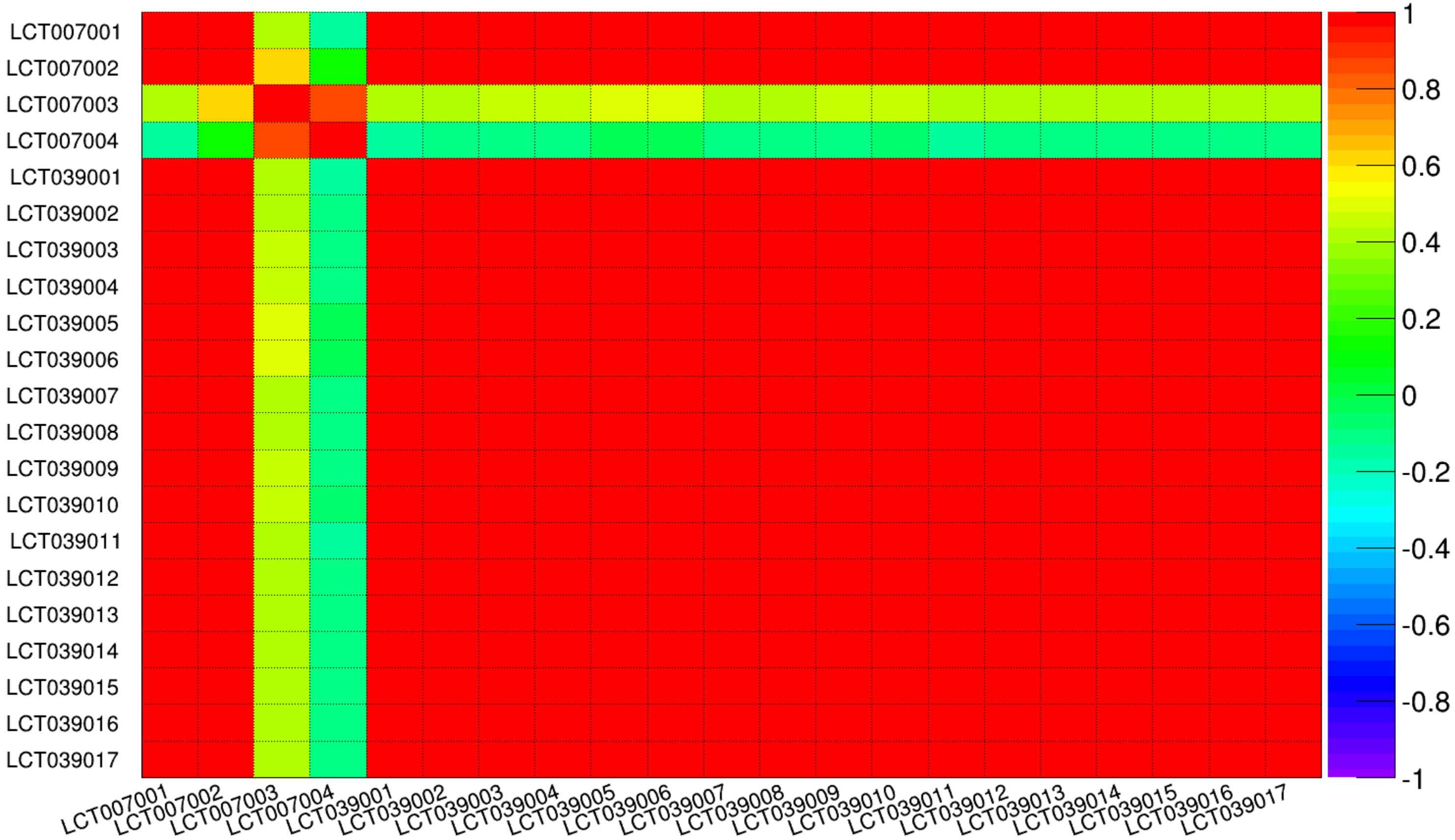
Reminder: Mean Value and Standard Deviation

- All mean values below $k_{eff} = 1$
  - Thus, with these k_{eff} values a bias of approx. -0.003 (+ uncertainty) can be expected
  - Standard deviations are between 1.1E-03 and 4.7E-03



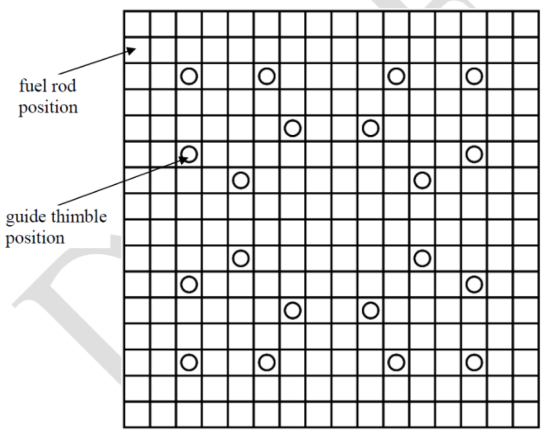
Reminder: Correlation Matrix

- High correlations up to almost 100% between benchmark experiments
  - However, two cases have significantly lower correlation coefficients

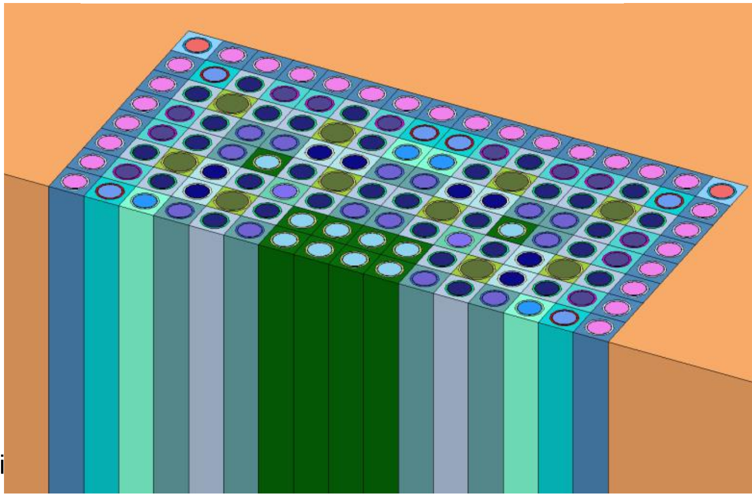


Benchmark Task & Application Case

- Benchmark task according to UACSA benchmark proposal:
  - Determination the computational bias for an application case in two ways:
    - Assuming, the 21 benchmark experiments are uncorrelated
    - Considering the correlation matrix derived from the common variation of shared uncertain parameters



- Application case:
  - Single 16×16-20 PWR UO_2 fuel assembly
  - Fully reflected by water
    - Achieved by modeling 60 cm of water around the fuel assembly in all directions
  - One sort of fuel pins with 5 wt.-% U-235 enrichment
  - Pitch of 1.43 cm
  - UO_2 density of 10.96 g/cm^3



Application Case Results

- The application case also run with SCALE‘s CSAS5 sequence
  - Configuration similar to the validation experiments
  - However, the convergence criterion was set to 2.0E-05

- Result for the neutron multiplication factor: 0.969979 ± 0.000020

- Result for the trending parameter EALF: 2.36489E-01 ± 1.83343E-05
  - This is within the range of EALF values from the validation pool:
    - Interpolation possible for the trending analysis

- TSUNAMI-3D-K5 result: 1σ k_{eff} uncertainty: 6.675E-03
  - Similar to the results from the validation pool

Trending Analysis

- χ^2-fit performed with RooFiLab (based on CERN's data analysis package ROOT)
- Assuming a linear fit function:

$$f(EALF) = a \times EALF + b$$

- Bias of the application case:

$$Bias_{app} = f(EALF_{app}) - 1.0$$

	Fit Options						
	Mean Values Only	k_{eff} Variances		k_{eff} Covariances		k_{eff} and EALF Covariances	
	Value	Value	Uncertainty	Value	Uncertainty	Value	Uncertainty
a [1/eV]	4.260E-04	2.385E-03	1.800E-02	-1.420E-03	3.900E-04	-5.179E-02	3.400E-04
b	9.969E-01	9.969E-01	3.400E-03	1.007E+00	4.300E-04	9.984E-01	1.200E-05
$k_{eff}(EALF_{app})$	9.970E-01	9.974E-01	5.314E-03	1.007E+00	4.390E-04	9.867E-01	7.806E-05
bias	-3.003E-03	-2.559E-03	5.314E-03	6.678E-03	4.390E-04	-1.335E-02	7.806E-05

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$k_{eff}(EALF_{app})$	9.970E-01	9.974E-01	5.314E-03	1.007E+00	4.390E-04	9.867E-01	7.806E-05
bias	-3.003E-03	-2.559E-03	5.314E-03	6.678E-03	4.390E-04	-1.335E-02	7.806E-05

bias as expected

bias changed sign

bias is factor ~4 larger than the expected value

Trending Analysis

- χ^2-fit performed with RooFiLab (based on CERN's data analysis package ROOT)
- Assuming a linear fit function:

$$f(EALF) = a \times EALF + b$$

- Bias of the application case:

$$Bias_{app} = f(EALF_{app}) - 1.0$$

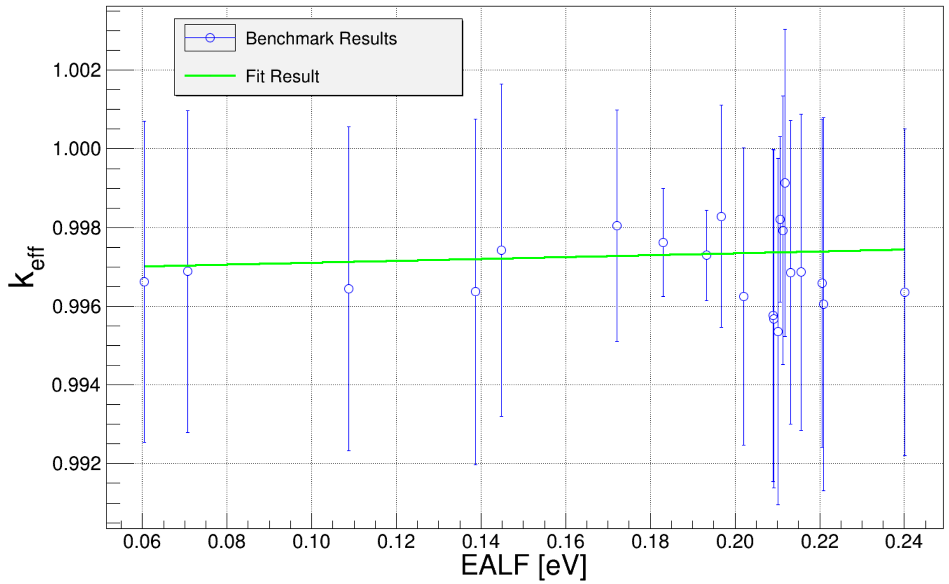
- Selecting experiments similar to the application case, i.e. choosing $EALF > 0.2$:

	Fit Options						
	Mean Values Only	k_{eff} Variances		k_{eff} Covariances		k_{eff} and EALF Covariances	
	Value	Value	Uncertainty	Value	Uncertainty	Value	Uncertainty
a [1/eV]	-2.977E-02	-3.196E-02	1.400E-01	-1.729E-02	1.100E-02	-4.367E-01	5.800E-03
b	1.003E+00	1.003E+00	3.000E-02	1.006E+00	1.100E-03	1.052E+00	6.100E-04
$k_{eff}(EALF_{app})$	9.962E-01	9.957E-01	4.369E-02	1.002E+00	2.727E-03	9.529E-01	1.450E-03
bias	-3.754E-03	-4.250E-03	4.369E-02	2.078E-03	2.727E-03	-4.707E-02	1.450E-03

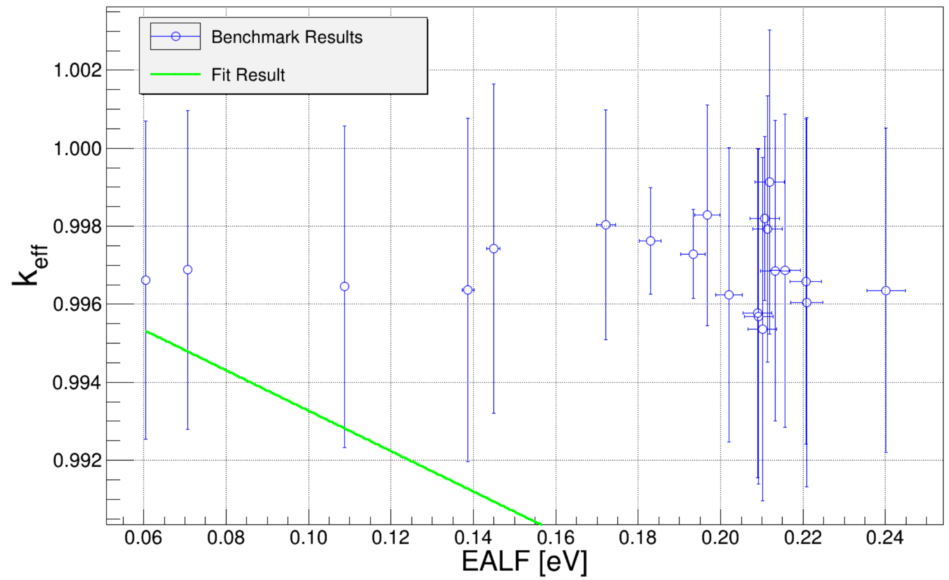
- The same qualitative behavior of the bias

Visualization of Results

- Variances only:



- Covariances in k_{eff} and EALF:



TSURFER Results

- Using the TSUNAMI results for the sensitivities on nuclear reactions
  - Testing the impact of different fit options and recommendations
  - Two sources of uncertainties: the SUnCISTT analysis and the ICSBEP values

- Assuming uncorrelated benchmark experiments:

Analysis ID	Uncertainty source	Additional configuration	Active benchmarks	Calculated k_{eff} value	Relative uncertainty	Relative Bias	Bias	Relative bias uncertainty	Adjusted k_{eff} value
I1	SUnCISTT		21/21	0.96879	0.689	-0.24051	-0.0023300	0.13029	0.97112
I2	SUnCISTT	off.-diag. corr. coeff. = 0	21/21			-0.24321	-0.0023562	0.13110	0.97115
I3	SUnCISTT	EALF > 0.2	12/21			-0.29536	-0.0028614	0.15500	0.97165
I4	ICSBEP		21/21			-0.26039	-0.0025226	0.10163	0.97131
I5	ICSBEP	EALF > 0.2	12/21			-0.30426	-0.0029477	0.10422	0.97174

- Neglecting correlations results in a similar bias even for different configurations
- Bias close to the expected value

TSURFER Results

- Using the TSUNAMI results for the sensitivities on nuclear reactions
  - Testing the impact of different fit options and recommendations
  - Two sources of uncertainties: the SUnCISTT analysis and the ICSBEP values

- Taking into account the correlations of k_{eff} from the SUnCISTT analysis:

Analysis ID	Uncertainty source	Additional configuration	χ^2/NDF cut	Active benchmarks	Calculated k_{eff} value	Relative uncertainty	Relative Bias	Bias	Relative bias uncertainty	Adjusted k_{eff} value
C1	SUnCISTT		1.2	7/21	0.96879	0.689	0.34209	0.0033142	0.22285	0.96548
C2	SUnCISTT	corr. coeff. < 0.95	1.2	20/21			0.081759	0.00079208	0.2287	0.968
C3	SUnCISTT		infinite	21/21			1.6414	0.015902	0.16339	0.95289
C4	SUnCISTT	EALF > 0.2	1.2	5/12			-0.024391	-0.0002363	0.20913	0.96903
C5	ICSBEP		1.2	2/21			-0.18643	-0.0018061	0.14659	0.9706
C6	ICSBEP		infinite	21/21			-1.2482	-0.012092	0.097195	0.98088

- Large variations in estimated bias (-0.012 $\rightarrow$ +0.016) and in adjusted k_{eff} value (0.953 $\rightarrow$ 0.981)

Discussion of Results

Discussion of Results for this example:

- The computational bias strongly depends on the configuration of the calculation method
- For the uncorrelated case, the two approaches under investigation yield similar results
- However, taking the correlations into account, for some configurations the adjustment procedure returns counterintuitive results
  - “known feature” of the χ^2-fit in case of very high correlations, other similar examples can be found in the literature.
- In the TSURFER approach, the variances assigned to each benchmark experiment have an impact on the result
  - The discrepancies found between the ICSBEP and the SUnCISTT results have to be resolved
- So far no conclusive determination of the bias, if correlations are included

Summary & Outlook

- The correlation matrices derived with GRS' SUnCISTT have been applied in the determination of the computational bias of an application case
- Two common procedures have been tested:
  - Trending analysis, using EALF as trending parameter
  - SCALE's TSUNAMI/TSURFER approach
- Results neglecting the correlations are in agreement
- Once correlations are introduced, the result depends on the configuration of the method in both cases

- The treatment of correlated benchmark experiments in the validation is a topic for further research
- The best practice to use uncorrelated benchmark experiments as basis for the validation pool avoids these challenges

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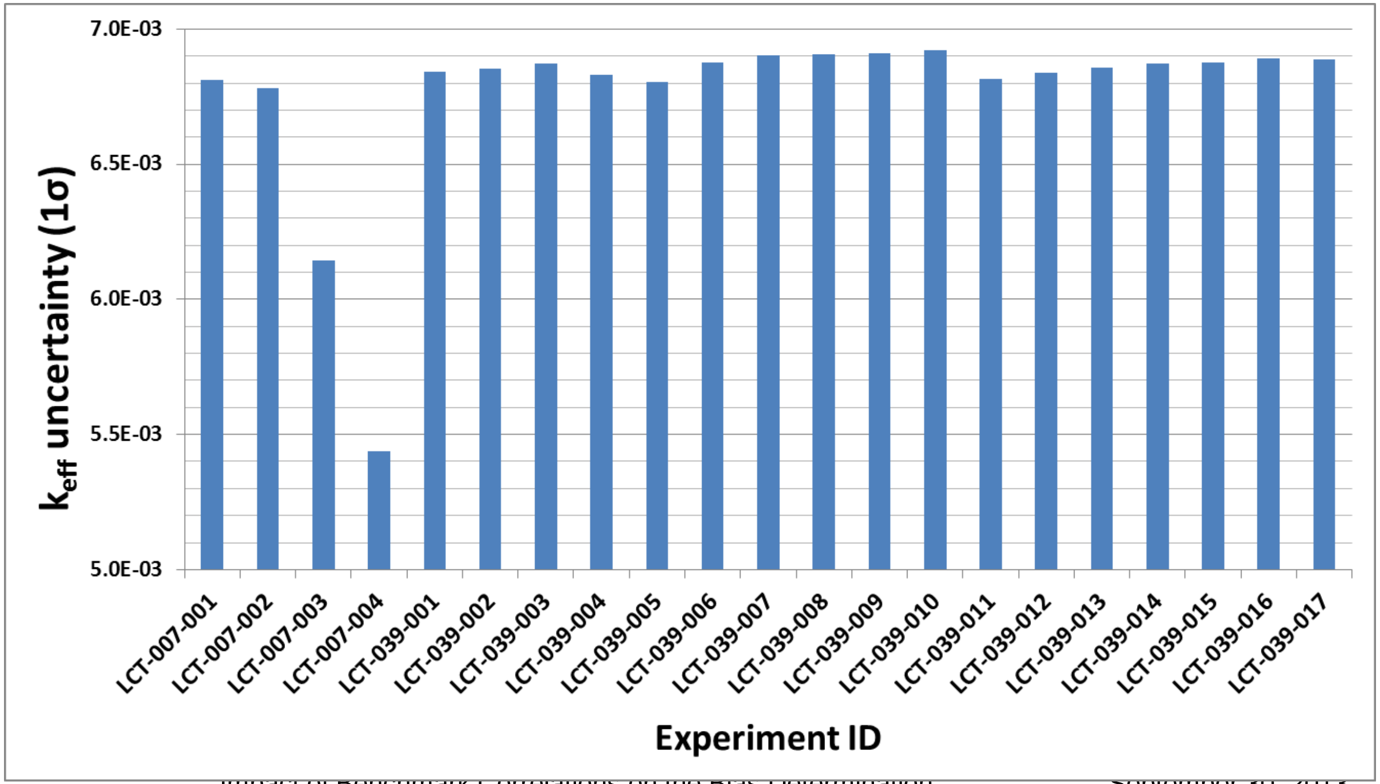
Comparison with TSUNAMI Results

- Analysis of uncertainties due to neutron cross-sections with the TSUNAMI-3D-K5 sequence of ORNL's SCALE program suite
  - TSUNAMI results needed for the bias determination with TSURFER
- Overall: the uncertainties are higher compared to the variation of the manufacturing tolerances
  - Similar trend for LCT-007-003 and LCT-007-004



Trending Analysis with EALF

- The benchmark experiments are correlated in the trending parameter EALF
- LCT-007-003/004 are highly correlated
- These correlations have to be taken into account in the trending analysis
- The RooFiLab tool provides the possibility to fit correlated parameters
    - It relies on the well established TMinuit algorithms in the ROOT framework