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Integral benchmarks for data assimilation: selection of a consistent set and establishment of integral correlations

Evgeny Ivanov, Tatiana Ivanova and Giulio-Emilio Bianchi

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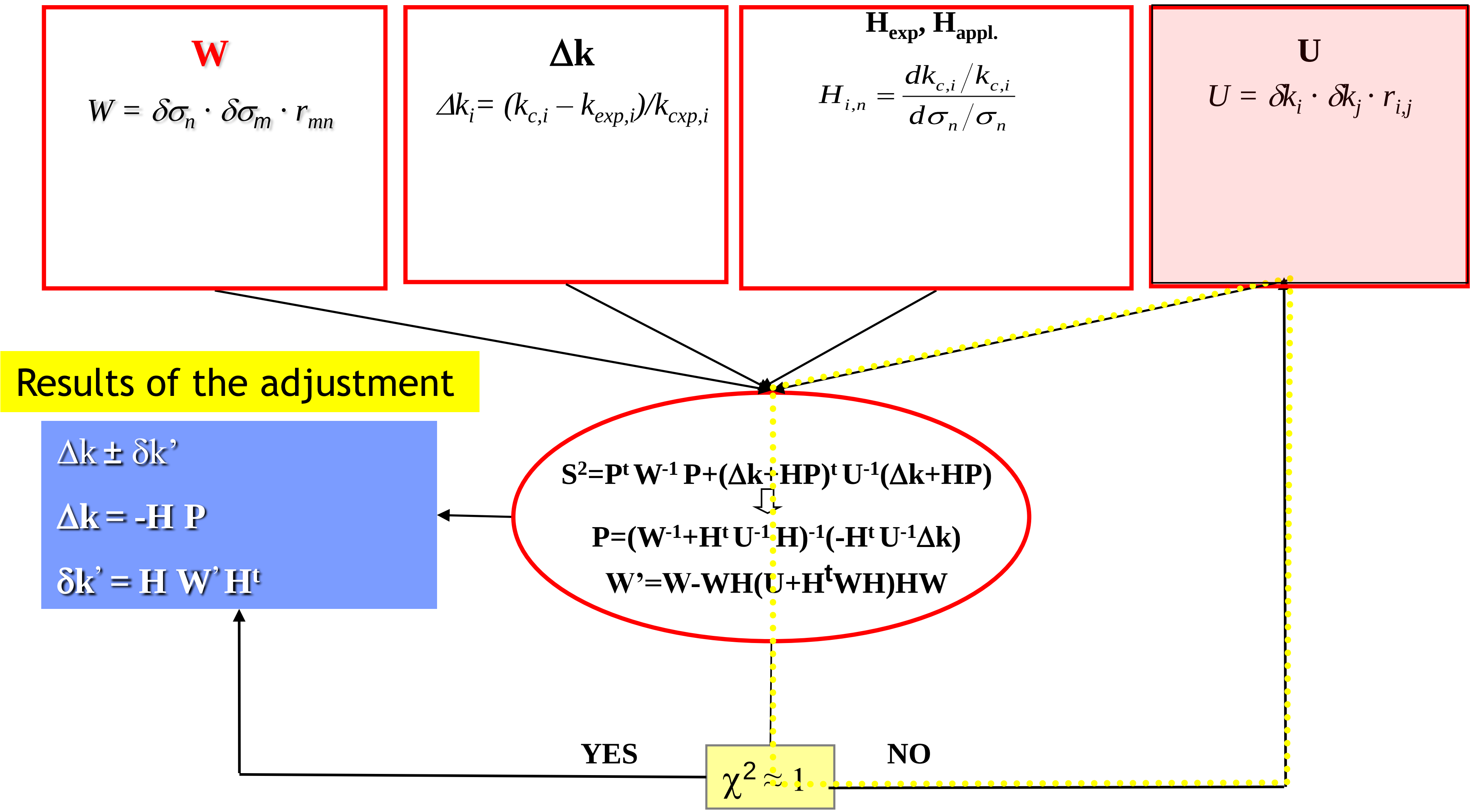
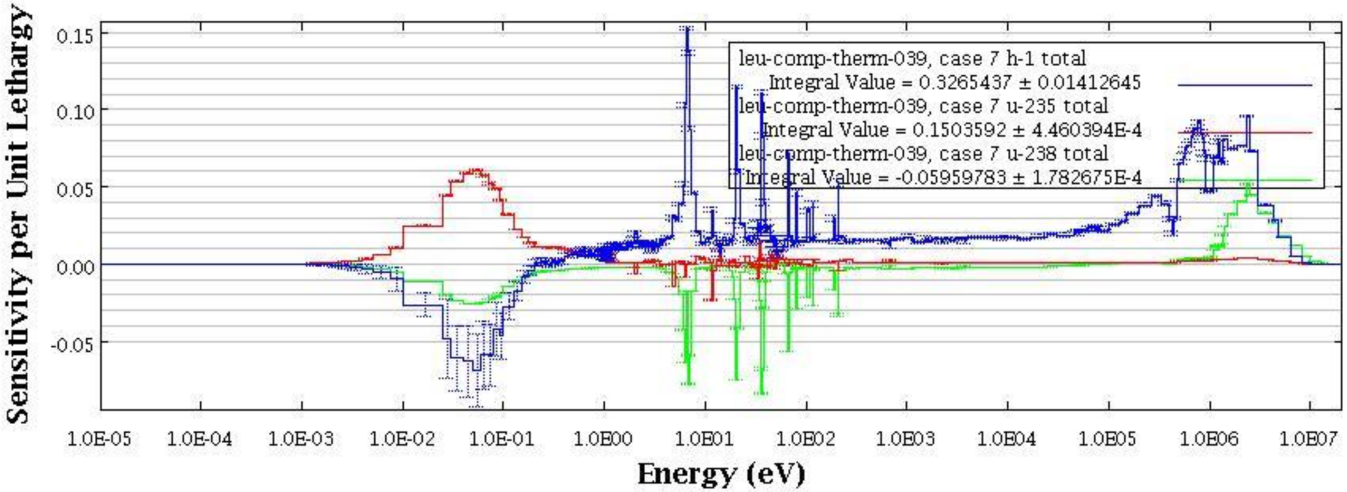
Outline

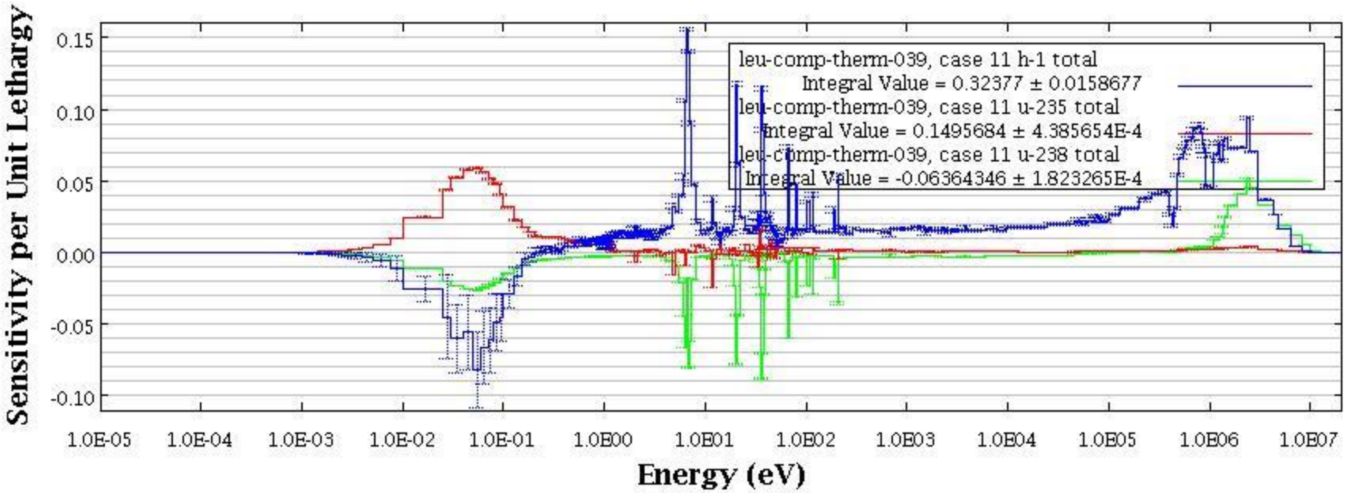
- Introduction: motivation and work status
- Oak Ridge spheres (HMF configurations issues) analysis for IRPhEP, CIELO demands
  - Sensitivity analysis
  - Equivalence studies
- Examples of correlations' impact
  - UACSA IV-th benchmark
  - Case description
  - Methodology
  - Results, discussion and lesson learned
- Further studies and conclusions

GLLSM procedure, k-eff example



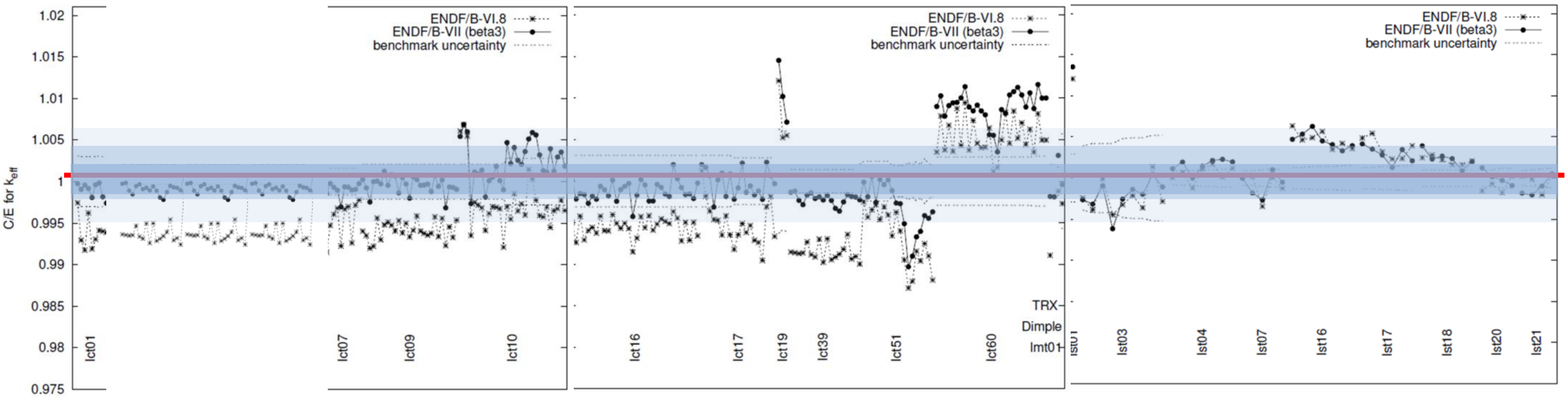
Sensitivity profiles for LCT-039





Example “Stress test” of validation procedure

Steven C. van der Marck, **Benchmarking ENDF/B-VII.0,**
Nuclear Data Sheets 107 (2006) 3061–3118



Attention: the results of validation can be user-dependent

$$d_m = \{\textstyle\sum_i (C-E)_i / s.d._i{}^2\} / \{\sum_i 1/s.d._i{}^2\}$$

$$s_m = \sqrt{\left[\sum_i {}^{[(C-E)_i - d_m]^2}\!/_{s.d._i{}^2}\right] / \left[\sum_i 1/s.d._i{}^2\right]}$$

TABLE XIX: The average values for $C/E-1$ (in pcm) for ENDF/B-VII.0 per main ICSBEP benchmark category.

	COMP				MET				SOL
	therm	inter	fast	mixed	therm	inter	fast	mixed	therm
LEU	17				−41				123
IEU	103	219					182		
HEU		1744		104	−51	88	147	812	108
MIX	428		110				193		−254
PU		1110				4565	229	936	620
U233	146						−364		66

Examples of impact of experimental uncertainties correlations

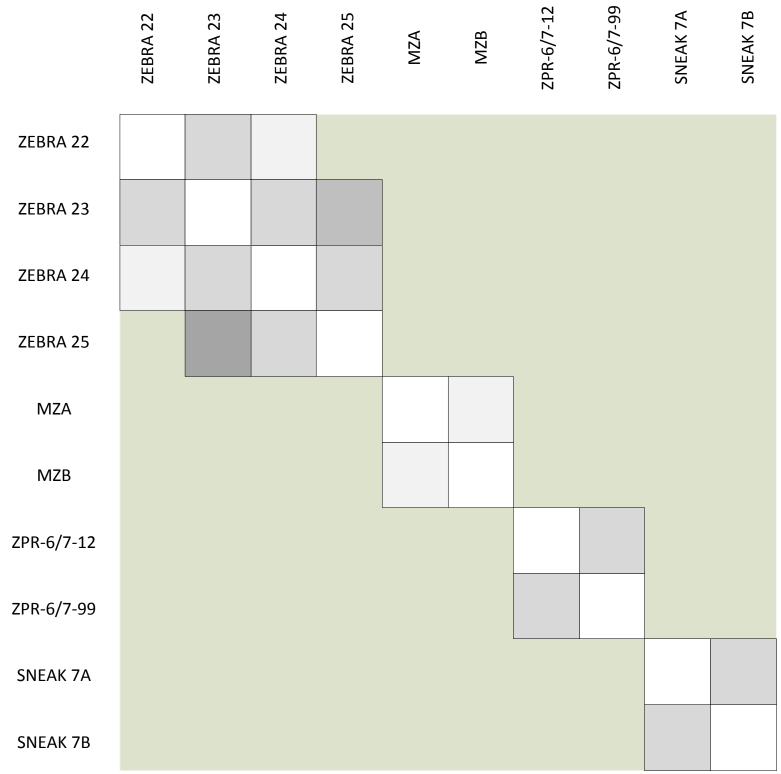
- Approach used to establish the correlations is proposed by IPPE

  T. Ivanova, M. Nikolaev, K. Raskach, E. Rozhikhin, A. Tsiboulia, "Influence of the Correlations of Experimental Uncertainties on Criticality Prediction", NSE, 145 (1), September 2003, pp. 97-104.

- Example of correlations for established at IRSN for a set of Mixed Plutonium-Uranium Oxide (MOX) fuelled configurations used for fast reactor applications:

Table 1 Characteristics of Selected Benchmarks [1]

Assembly	V, litres	Pu, at%	σ, %
ZEBRA22	2261.3	18	0.18
ZEBRA23	2373.7	18	0.18
ZEBRA24	2434.2	18	0.18
ZEBRA25	2552.3	18	0.18
MZA	2256.0	18	0.19
MZB	7110.4	18	0.13
ZPR-6/7-12	12478.7	19	0.23
ZPR-6/7-99	11678.8	11	0.22
SNEAK7A	453.6	8	0.29
SNEAK7B	1260.6	8	0.35



*Correlations for ZEBRA are established by John Rowlands

Correlation in experimental uncertainties impact (CIELO Conf, Nov, 2013)

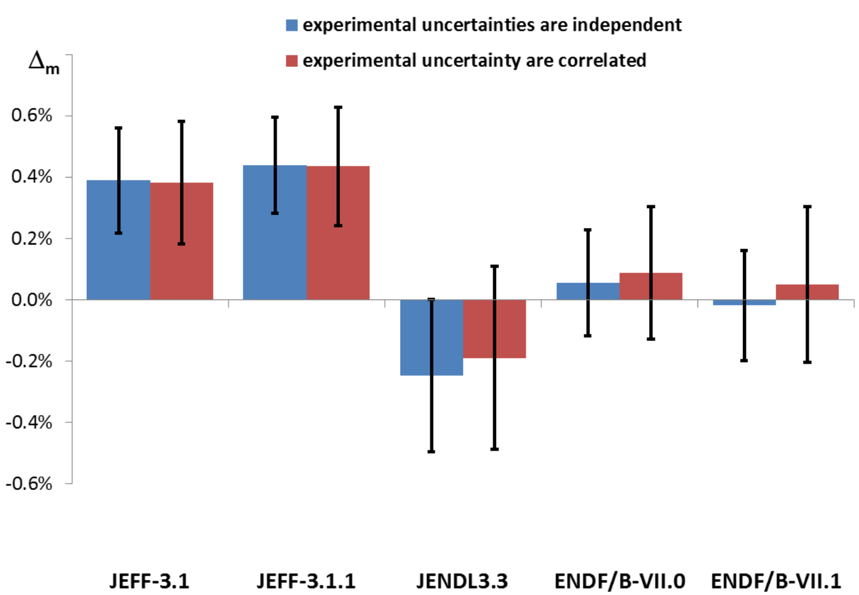
$$\hat{C} = \vec{\sigma}_C^T \cdot \hat{I} \cdot \vec{\sigma}_C + \vec{\sigma}_E^T \cdot \hat{V} \cdot \vec{\sigma}_E$$

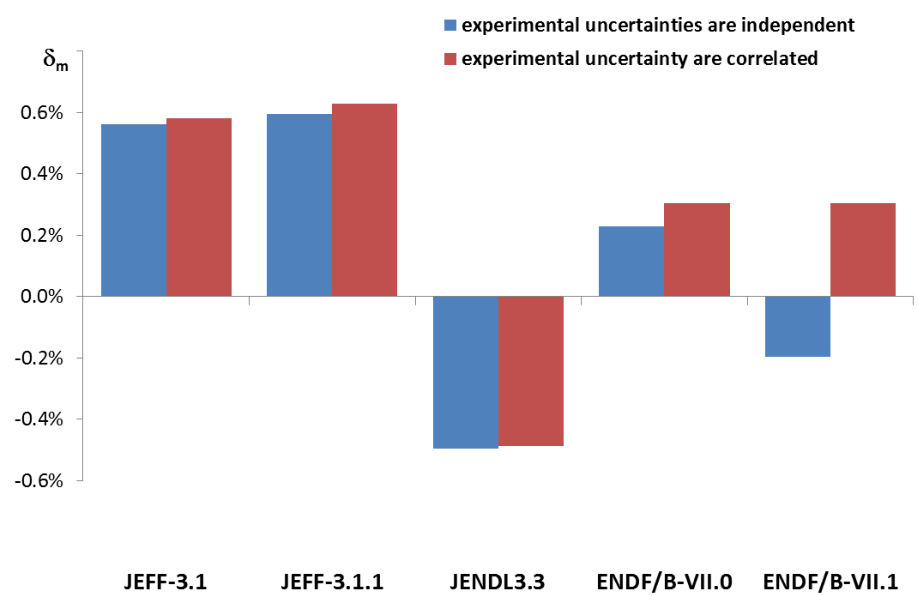
$$\vec{\Delta} = \left\| \hat{C} \right\| \cdot \left\| \hat{C}^{-1} \cdot (\vec{k}_C - \vec{k}_E) \right\|$$

$$\vec{\sigma}^2 = \left\| \hat{C} \right\| \cdot \left[((\vec{k}_C - \vec{k}_E) - \vec{\Delta})^T \cdot \hat{C}^{-1} \cdot ((\vec{k}_C - \vec{k}_E) - \vec{\Delta}) \right]$$

An expectation of an ultimate bias, i.e. bias + uncertainty could be recommended as figure of merit for conservative approach

$$\delta_m = \Delta_m + \sigma_m \cdot \Delta_m \cdot \left| \Delta_m \right|^{-1}$$





^{235}U spheres, Problem characterization

Table 4-1. Sample Results for the Detailed Benchmark Model, ENDF/B-VII.0.

Model	Benchmark			Calculated							
				MCNP5 ENDF/B-VII.0(a)			$\frac{C-E}{E}^{(d)}$	KENO-VI ENDF/B-VII.0(b,c)			$\frac{C-E}{E}^{(d)}$
	k_{eff}	±	σ	k_{eff}	±	σ		k_{eff}	±	σ	
Case 1	1.0024	±	0.0007	1.00373	±	0.00002	0.13%	TBD			
Case 2	0.9964	±	0.0007	0.99821	±	0.00002	0.18%	TBD			

(a) Results obtained using 500,000 histories for 2650 cycles, skipping the first 150 cycles.
(b) Results provided by John D. Bess from Idaho National Laboratory.
(c) Results obtained using TBD histories for TBD cycles, skipping the first TBD cycles.
(d) 'E' is the expected or benchmark value. 'C' is the calculated value.

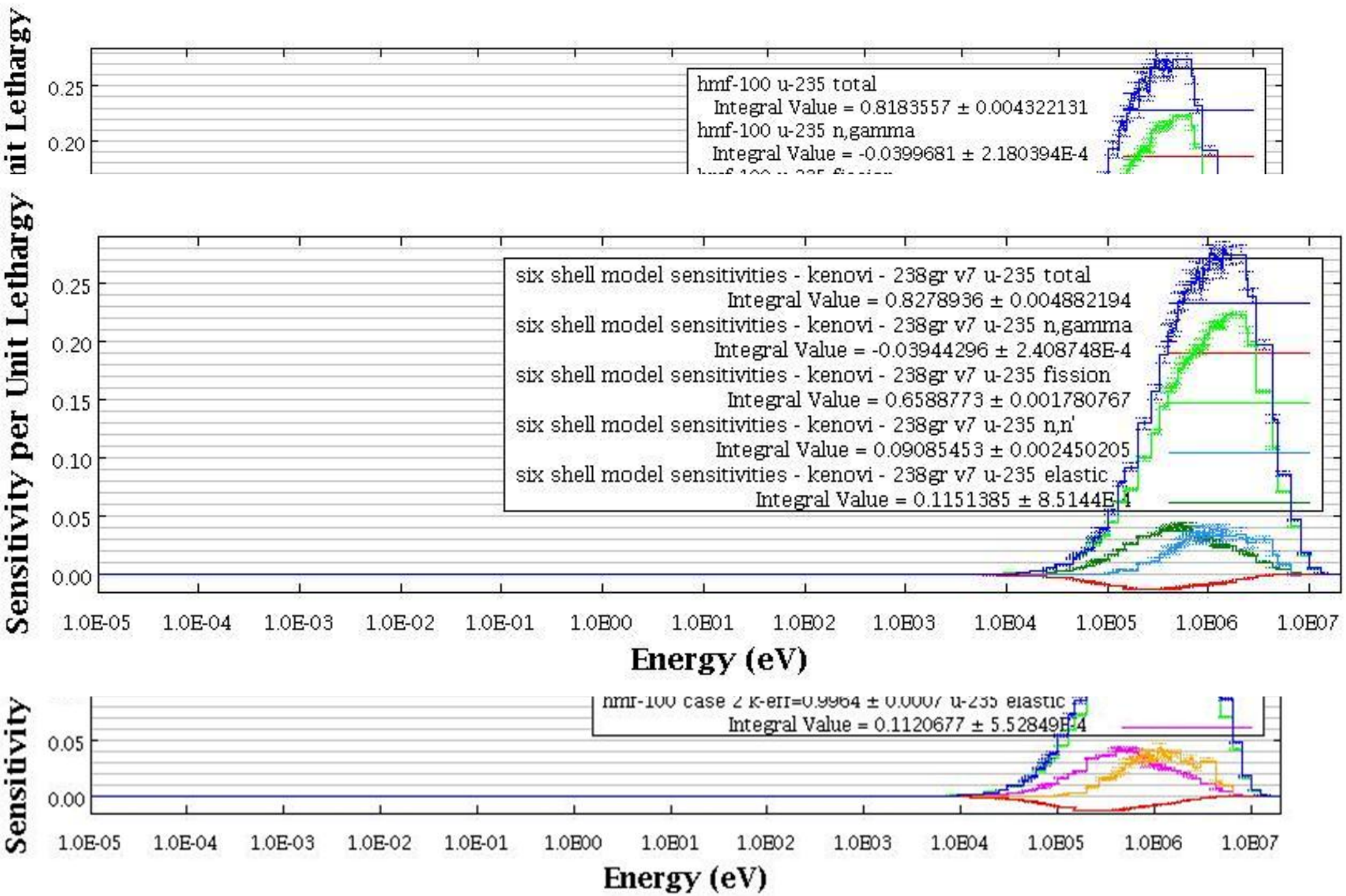
Table 4-2. Sample Results for the Simple Benchmark Model, ENDF/B-VII.0.

Model	Benchmark			Calculated							
				MCNP5 ENDF/B-VII.0(a)			$\frac{C-E}{E}^{(d)}$	KENO-VI ENDF/B-VII.0(b,c)			$\frac{C-E}{E}^{(d)}$
	k_{eff}	±	σ	k_{eff}	±	σ		k_{eff}	±	σ	
Case 1	1.0030	±	0.0007	1.00441	±	0.00002	0.13%	TBD			
Case 2	0.9964	±	0.0007	0.99828	±	0.00002	0.19%	TBD			

(a) Results obtained using 500,000 histories for 2650 cycles, skipping the first 150 cycles.
(b) Results provided by John D. Bess from Idaho National Laboratory.
(c) Results obtained using TBD histories for TBD cycles, skipping the first TBD cycles.
(d) 'E' is the expected or benchmark value. 'C' is the calculated value.

KENO-Va	k_{eff}	σ
ORSphere 1	1.005421	0.000119
ORSphere 2	0.999318	0.000117

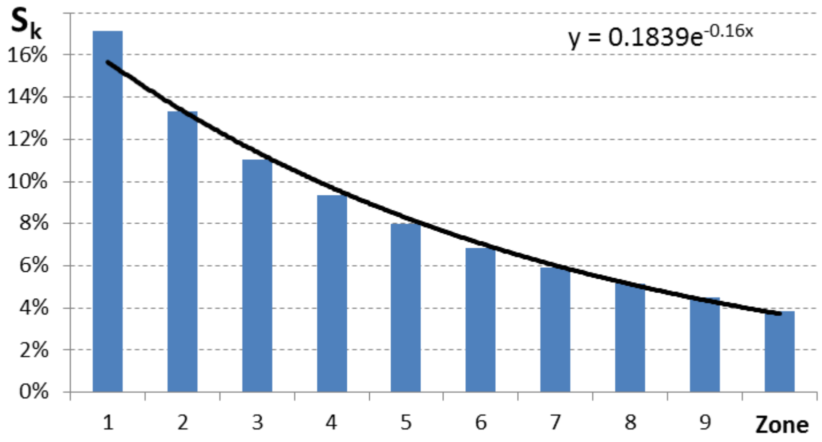
Sensitivity profiles for ORSphere cases 1 and 2 and for GODIVA



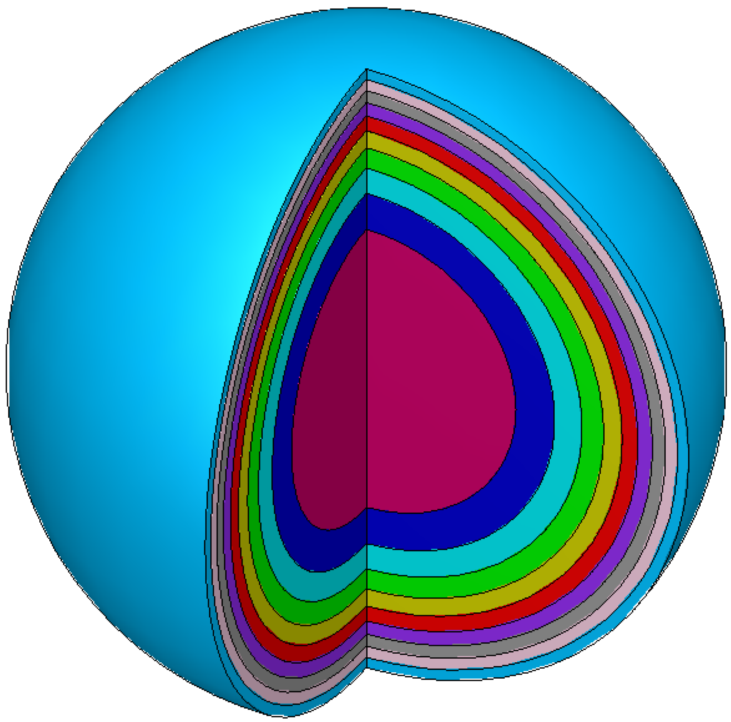
Influence of ^{235}U non-homogeneity

k_{eff} sensitivity

	Mass	Radius
ORSphere1	*84.7%*	*-90.1%*
ORSphere2	*85.1%*	*-90.6%*

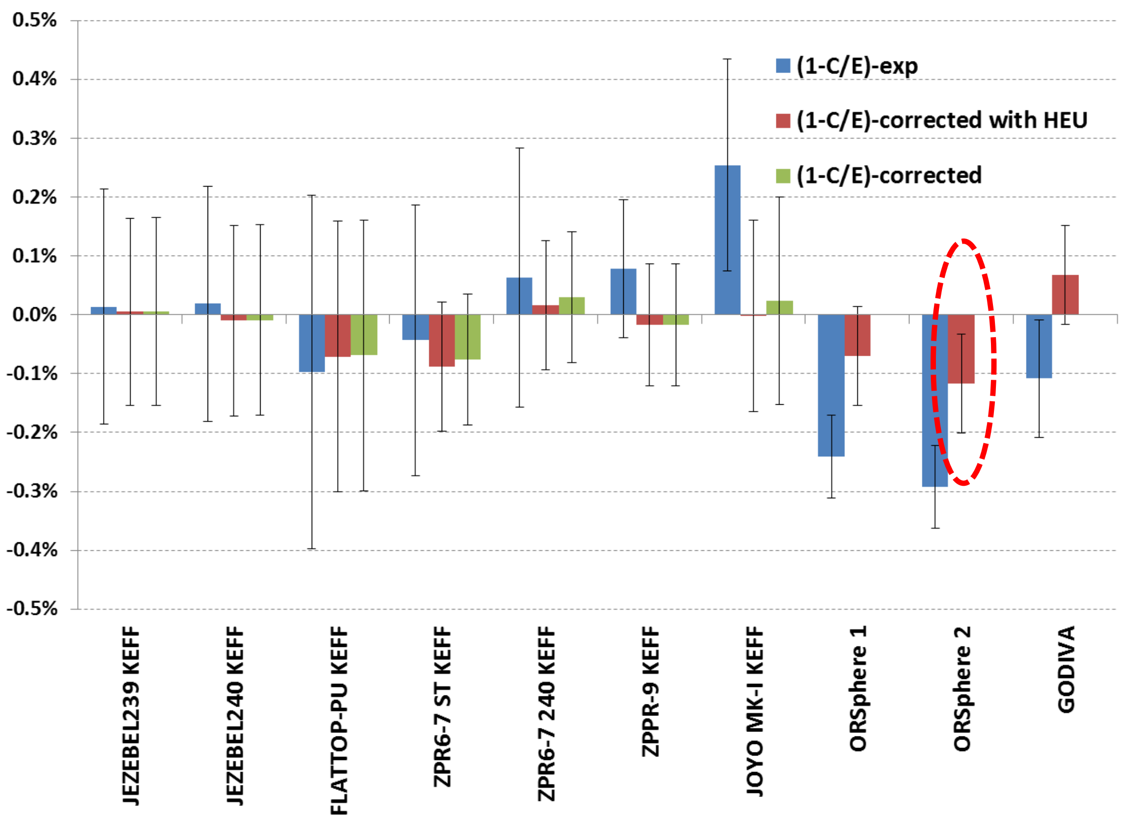


$\Delta\rho$=**0.2%** in central part with $\Delta\rho$**=-0.2%** on periphery gives **~75** pcm



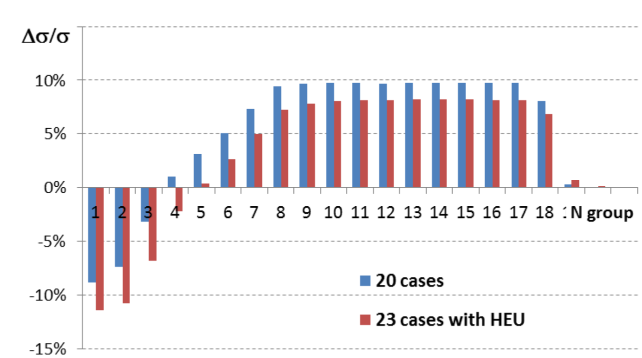
Scheme of division of the sphere by radiuses with the same volumes

^{235}U benchmarks' contribution in the results of data assimilation

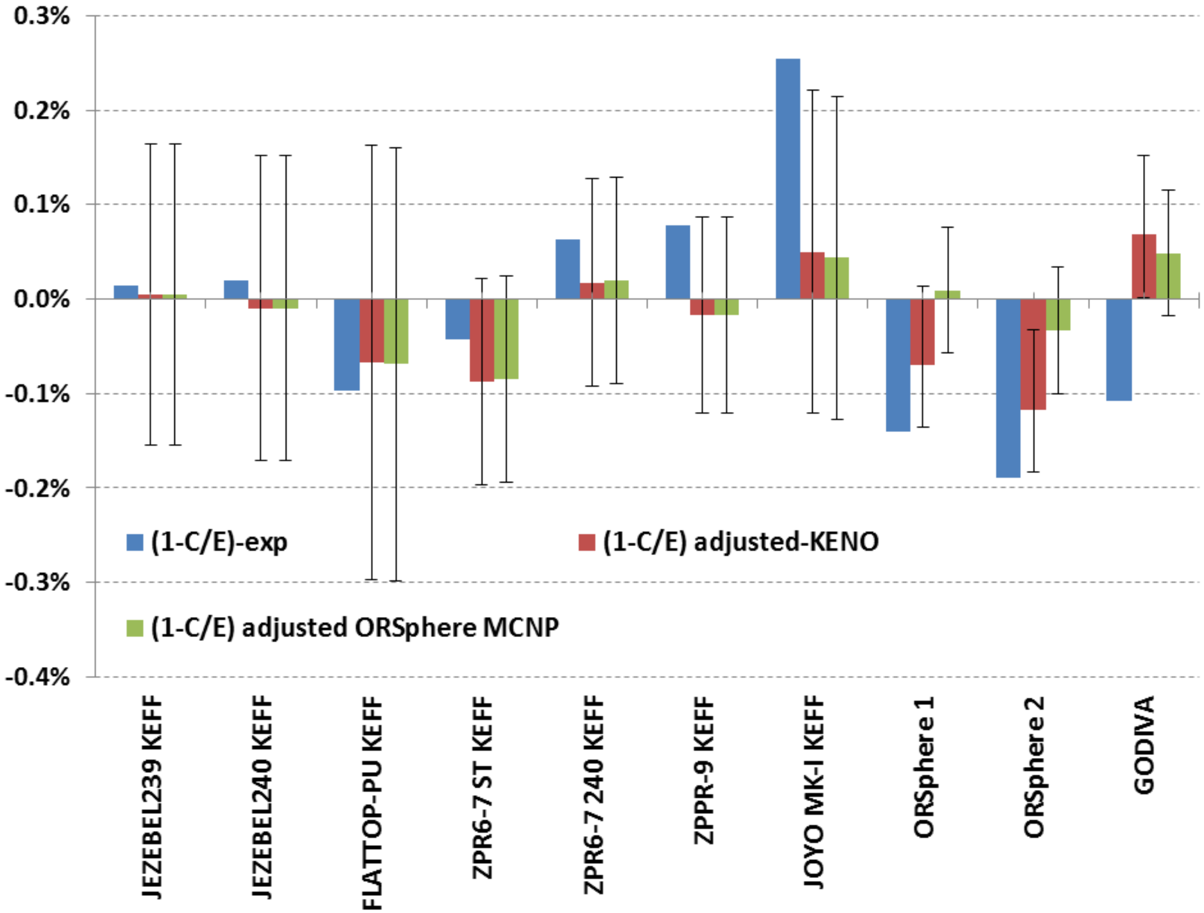


χ^2=0.778±0.393

^{235}U capture recommended correction



^{235}U benchmarks' contribution in the results of data assimilation



ENDF.B-VII.0

KENO-Va (238 gr)

$\chi^2=0.778\pm0.393$

with MCNP5 for ORSpheres

$\chi^2=0.757\pm0.345$

ORSpheres, experimental data “macroscopic” analysis

Basic notes:

•Two cores to be equivalent should have the same size in terms of neutron pass length

•Two cores of different size and the same shape are equivalent if the densities ratio has the same proportion as the sizes

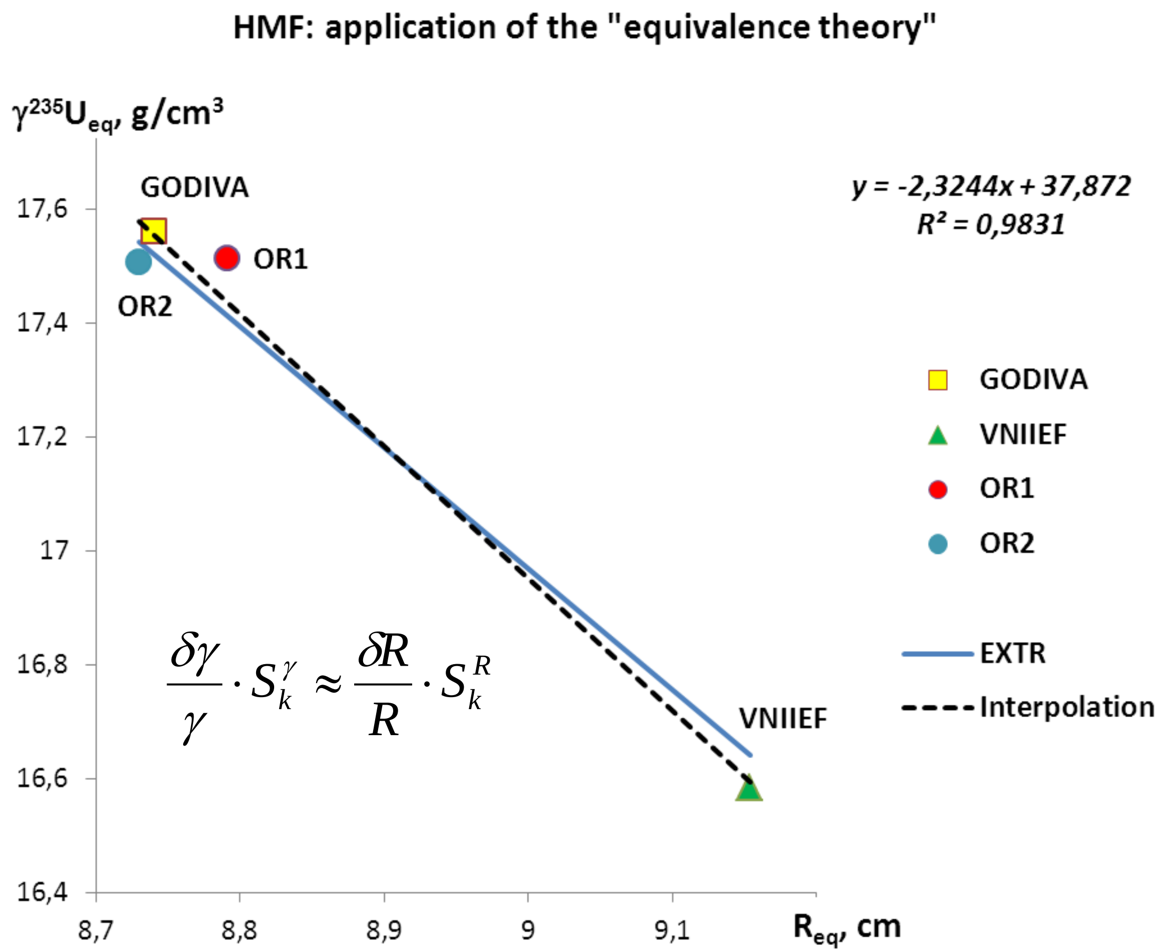
Application to benchmarks selection

•High enriched spheres do not lay on the same line

1.Errors in evaluations (unlikely)

2.Uncertain approach to criticality (+ kinetic parameters)

3.Fission phenomena (reported in different publications ***[V.Maslov], [N.Kornilov]*** and ***[L.Leal, G.Noguere]***)



$$\frac{\delta\gamma}{\gamma}\cdot S_k^{\gamma} \approx \frac{\delta R}{R}\cdot S_k^{R}$$

UACSA IV-th benchmark: ‘Homogeneous’ (LCT007 and 039) and ‘non-homogeneous’ lattices of cases (LCT 039)

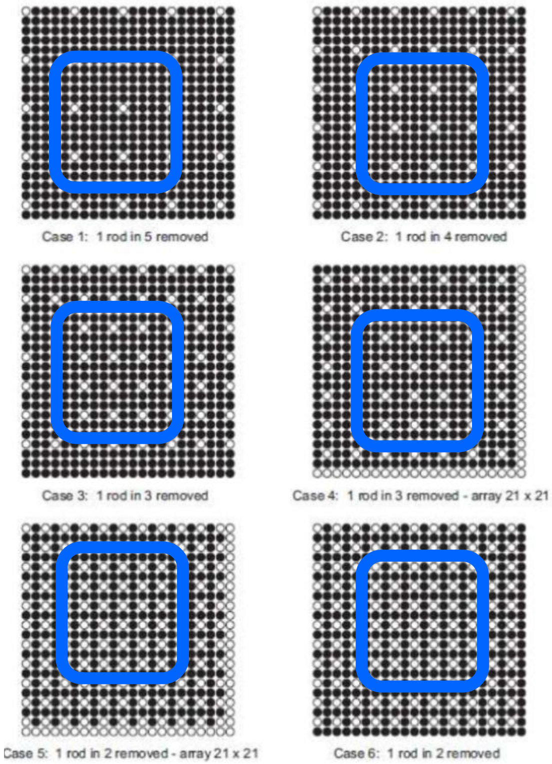
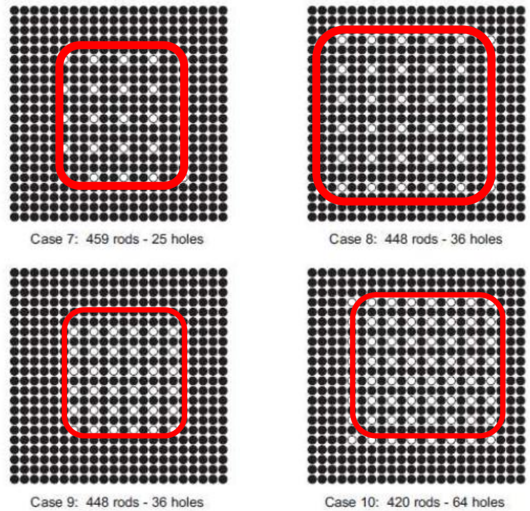


Figure 3: Cases 1-6 from LCT 039



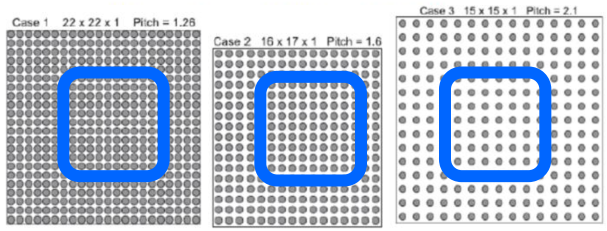


Figure 2: Cases 1-3 from LCT 007

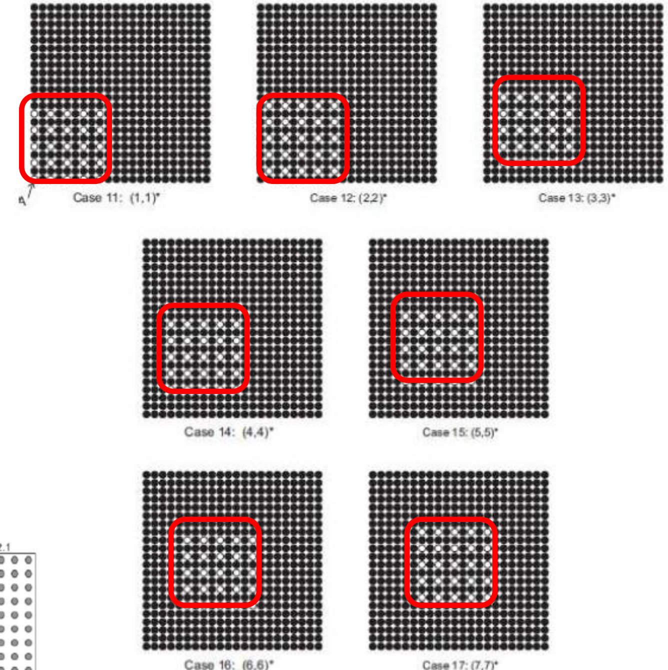
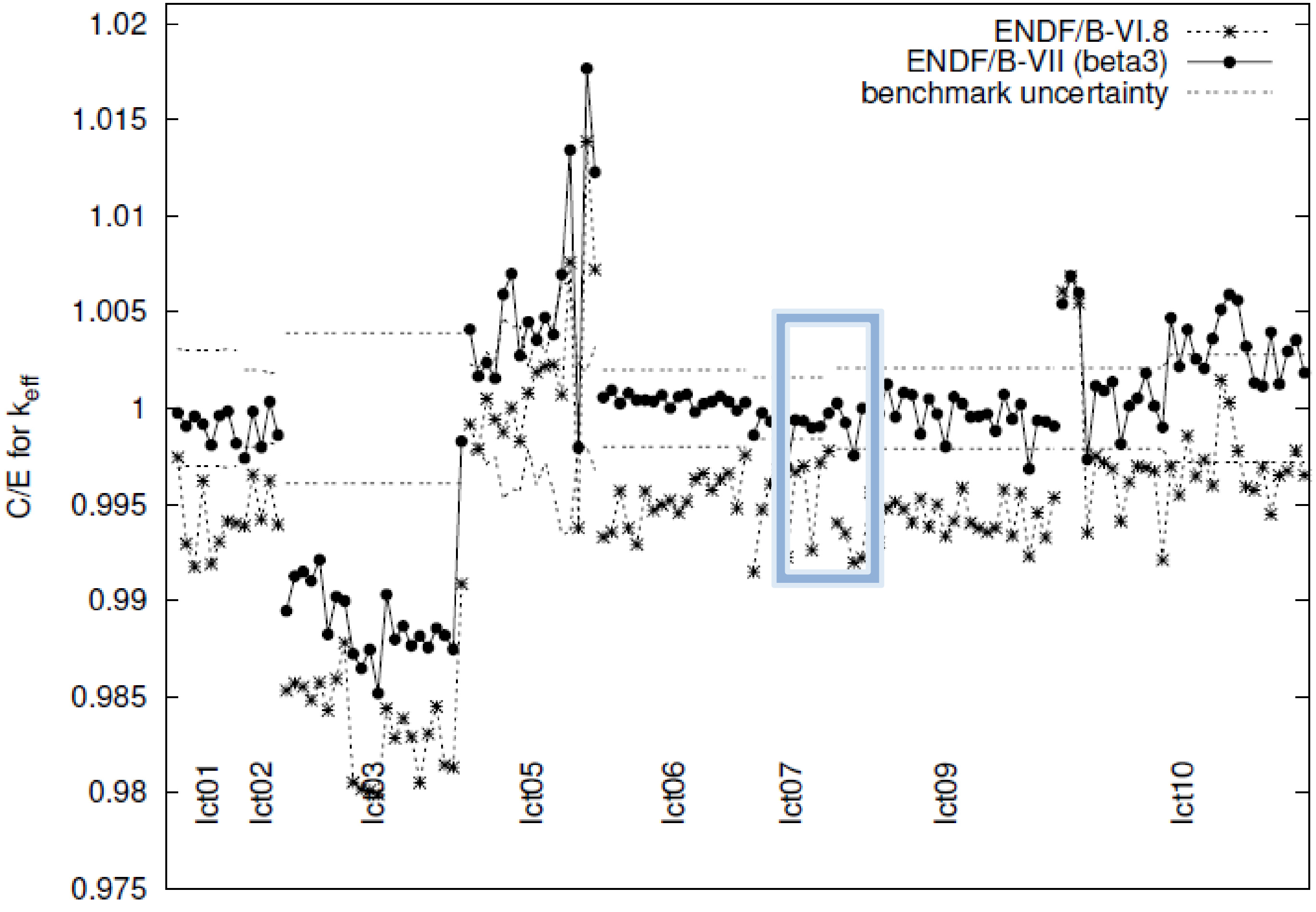


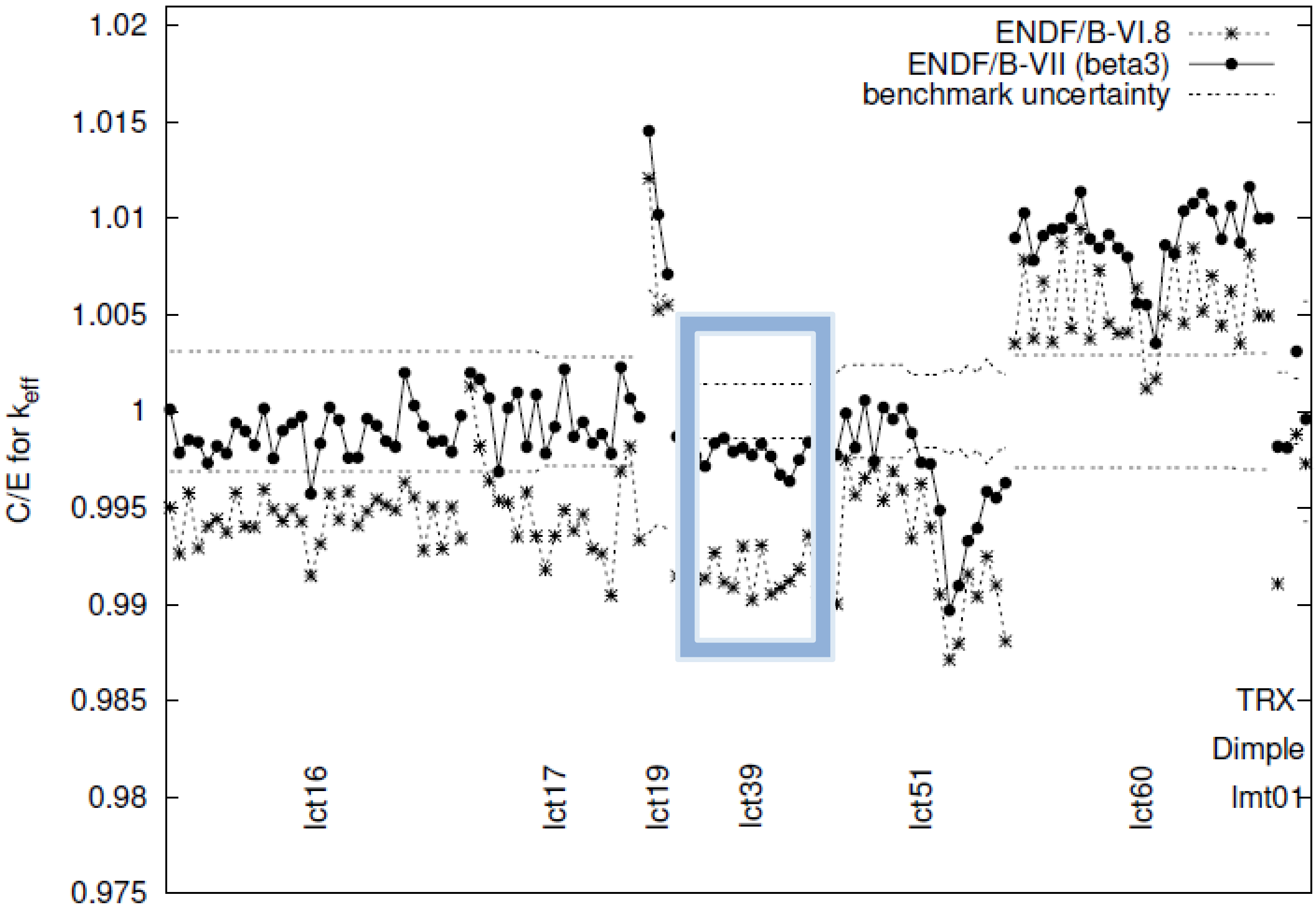
Figure 5: Cases 11-17 from LCT 039

Several SCALE/TSUNAMI-3D input desks by Ian Hill (OECD/NEA) were used

Results for LCT-007 benchmarks vs. all LCT benchmarks



Results for LCT-039 benchmarks vs. all LCT benchmarks



Results for LCT-039 and 007 benchmarks vs. all LCT cases

Steven C. van der Marck, **Benchmarking ENDF/B-VII.0,**
Nuclear Data Sheets 107 (2006) 3061–3118

TABLE XVIII: The number of benchmarks per main ICSBEP category for thermal/intermediate/fast/mixed neutron spectrum.

	COMP				MET				SOL	total
	therm	inter	fast	mixed	therm	inter	fast	mixed	therm	
LEU	257				1				49	307
IEU	6	4					16			26
HEU		6		1	41	5	66	5	87	211
MIX	34		1				4		10	49
PU		1				1	7	6	105	120
U233	8						4		5	17
total	305	11	1	1	42	6	97	11	256	730

TABLE XIX: The average values for $C/E-1$ (in pcm) for ENDF/B-VII.0 per main ICSBEP benchmark category.

	COMP				MET				SOL
	therm	inter	fast	mixed	therm	inter	fast	mixed	therm
LEU	17				−41				123
IEU	103	219					182		
HEU		1744		104	−51	88	147	812	108
MIX	428		110				193		−254
PU		1110				4565	229	936	620
U233	146						−364		66

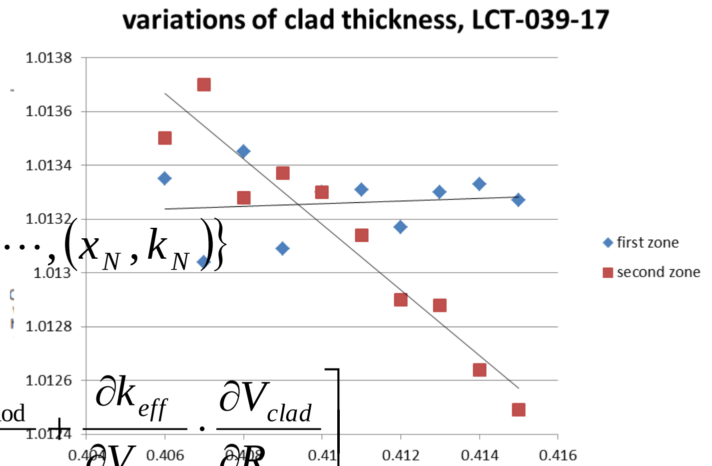
Sensitivity coefficients calculations, deterministic approach

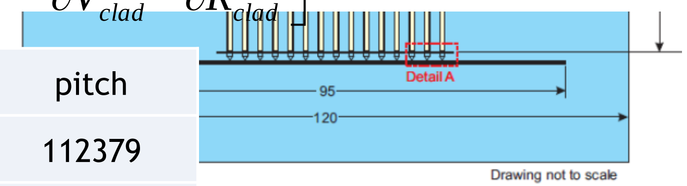
- Pin diameter
- Clad thickness
- Pellet density
- Enrichment
- Impurities
- Pitch
- Water height

$$k_{eff} \approx k_0 + \frac{\partial k}{\partial X} \cdot (X - X_0)$$

$$\left. \begin{array}{c} k_0 \\ \frac{\partial k}{\partial X} \end{array} \right\} \Leftarrow linear\,regression\{(x_1, k_1), (x_2, k_2), \cdots, (x_N, k_N)\}$$

$$S_{RAD:} = \frac{R_{clad}}{k_{eff}} \cdot \frac{\partial k_{eff}}{\partial R_{clad}} \approx \frac{R_{clad}}{k_{eff}} \cdot \left[\frac{\partial k_{eff}}{\partial V_{\mathrm{mod}}} \cdot \frac{\partial V_{\mathrm{mod}}}{\partial R_{clad}} + \frac{\partial k_{eff}}{\partial V_{clad}} \cdot \frac{\partial V_{clad}}{\partial R_{clad}} \right]$$



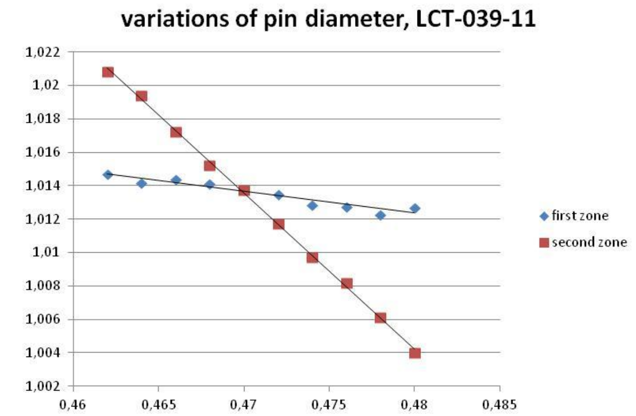


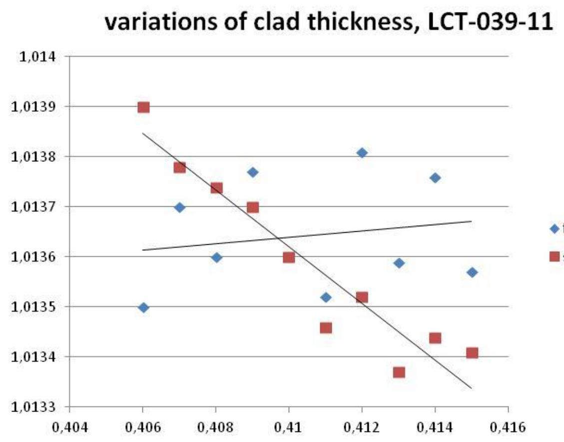
LCT-39-11	diameter	thickness	density	enrichment	impurity	pitch
OPT	-49713	-2858	9841	15021	-24	112379
DIRECT	-49999	-2057	7739	15893	-29	86461

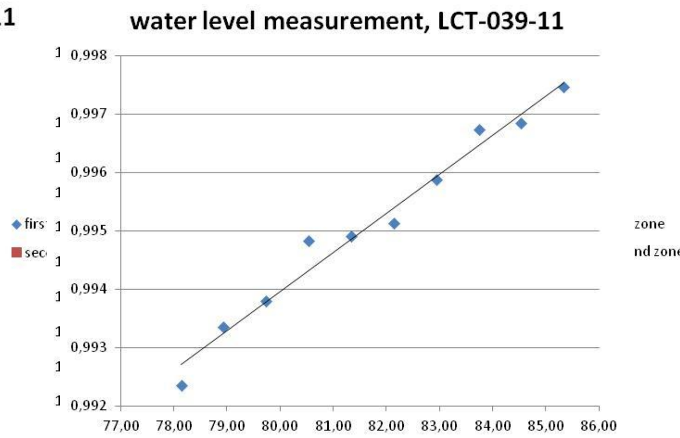
LCT-39-13	diameter	thickness	density	enrichment	impurity	pitch
OPT	-47676	-3051	10600	15410	-24	109968
DIRECT	-49340	-3755	9170	14873	-26	86554

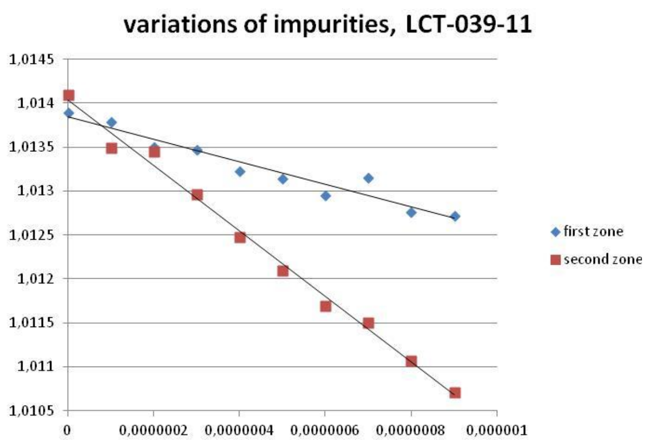
Computations were performed with SCALE-6.1/KENO-Va with ENDF/B-VII.0, and TSUNAMI-3D

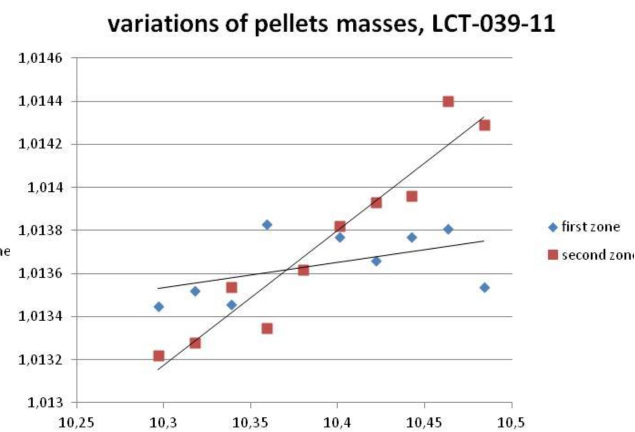
Examples of parametric studies, LCT-039-11

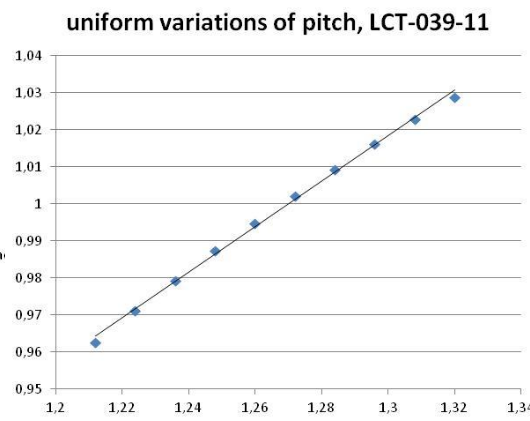












Note: bars of calculational standard deviations of each single k_{eff} are smaller than even markers

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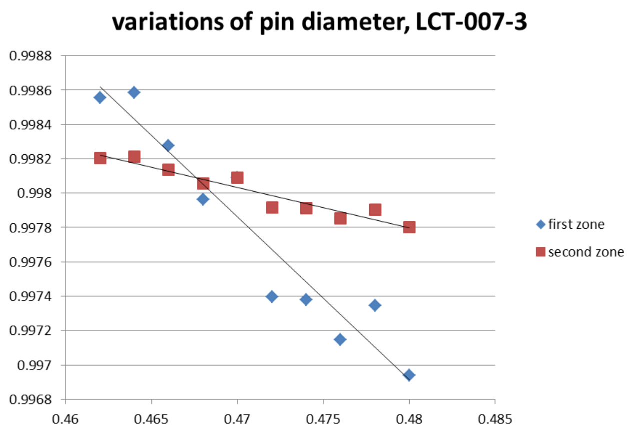
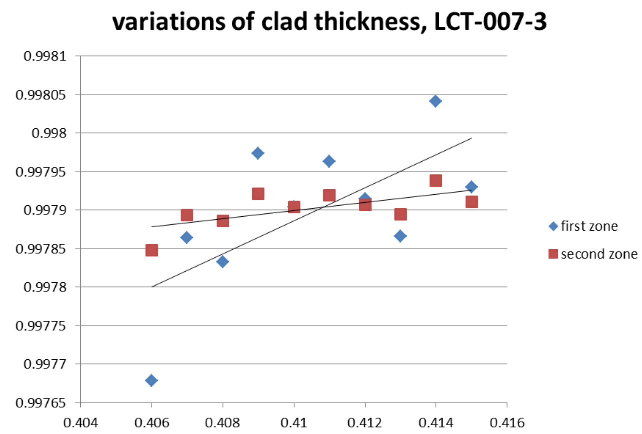
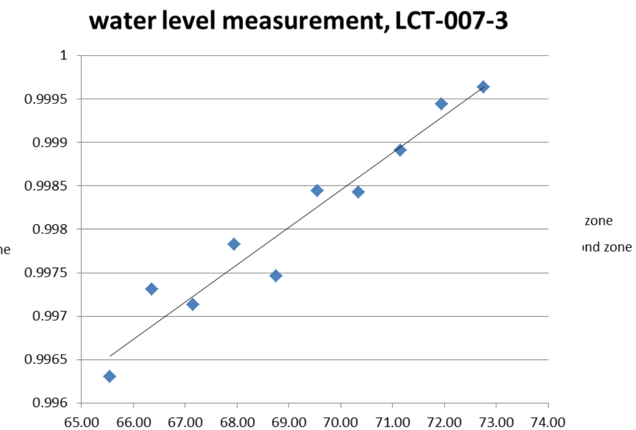
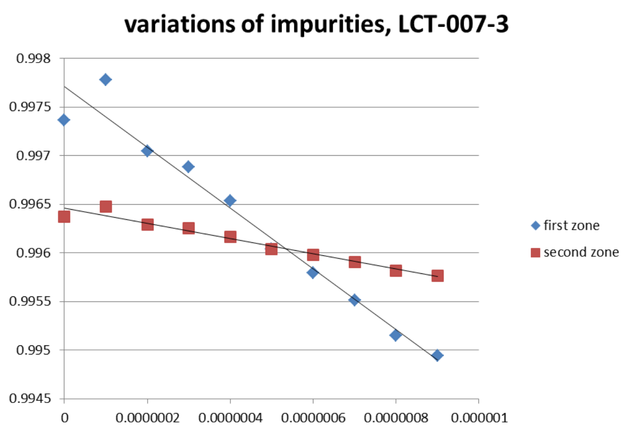
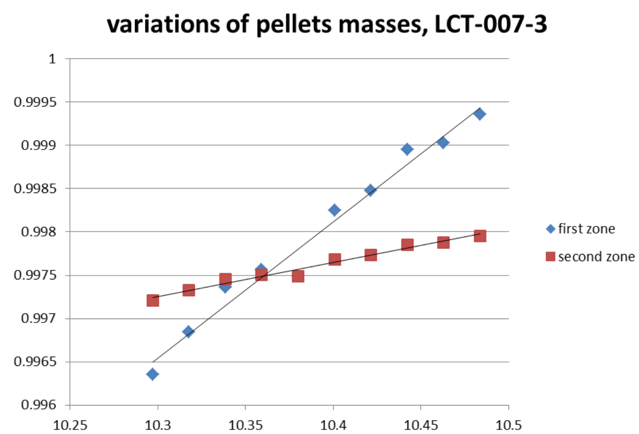
Examples of parametric studies, LCT-007-3

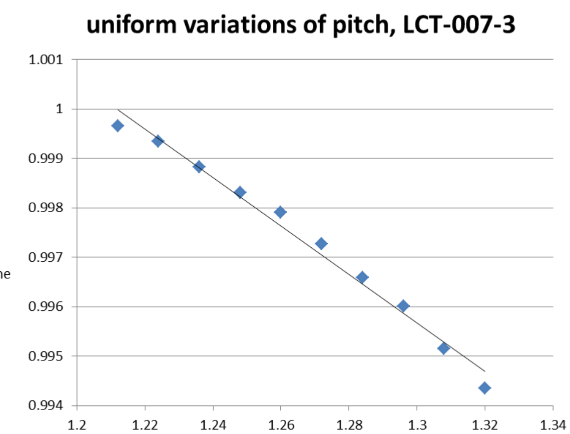






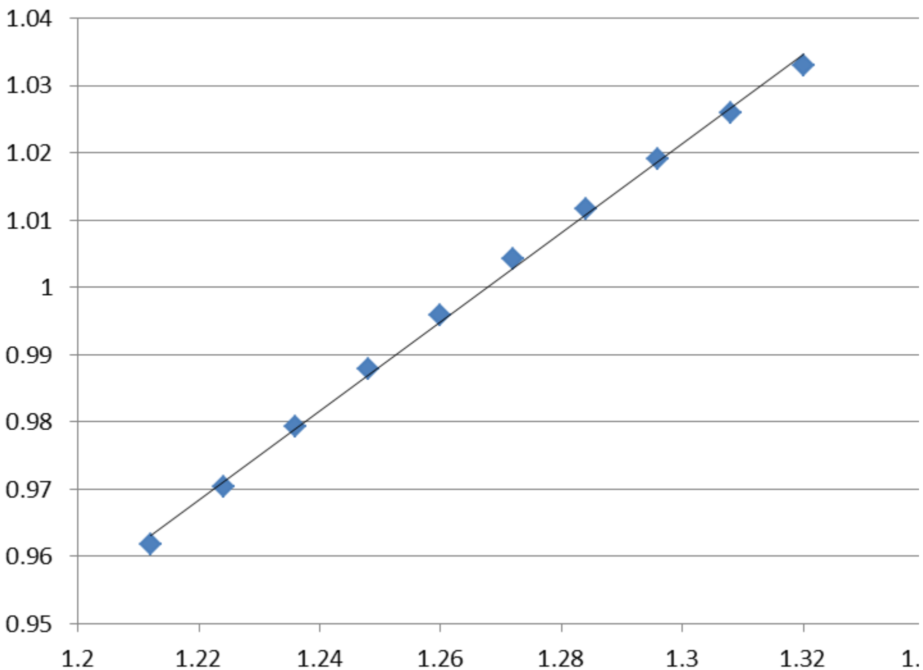




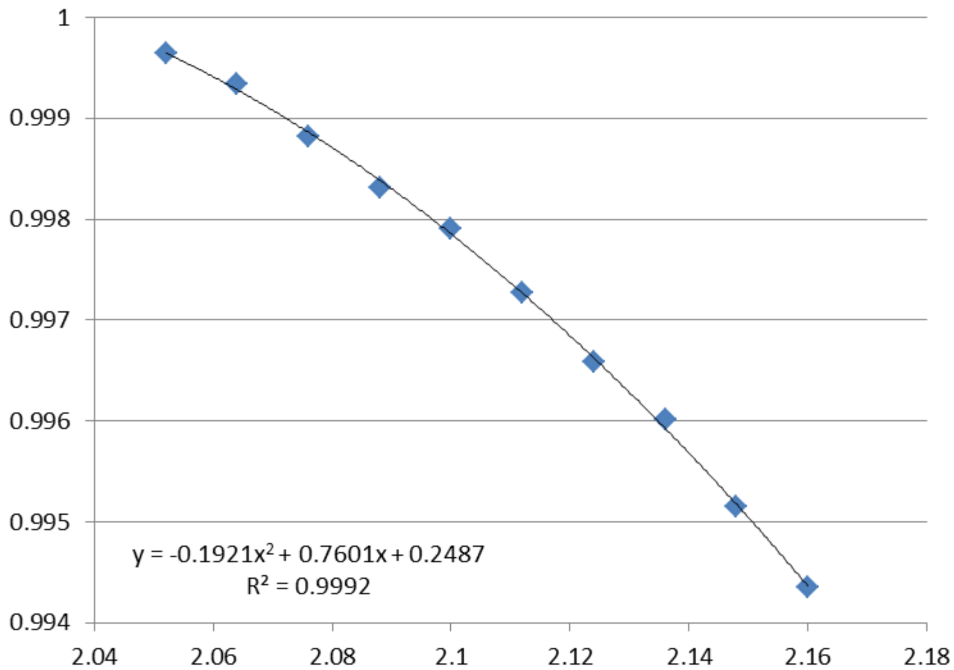


Under- vs over-moderated lattices (LCT-007-1 vs -3)

uniform variations of pitch, LCT-007-1



uniform variations of pitch, LCT-007-3



	Pin size	Clad size	Mass	Impurities	Enrichment	Pitch	Critical level
LCT-007-001	-2646.3±22.6	-158.37±19.1	361.4±26.5	-1.3±0.0	538.94±132.5	**83365.5±1301**	3350.0±614.5
LCT-007-003	-240.5±24.7	47.55±18.6	879.3±49.4	-1.0±0.0	1028.34±43.4	**-10273.1±438.5**	6693.3±583.5

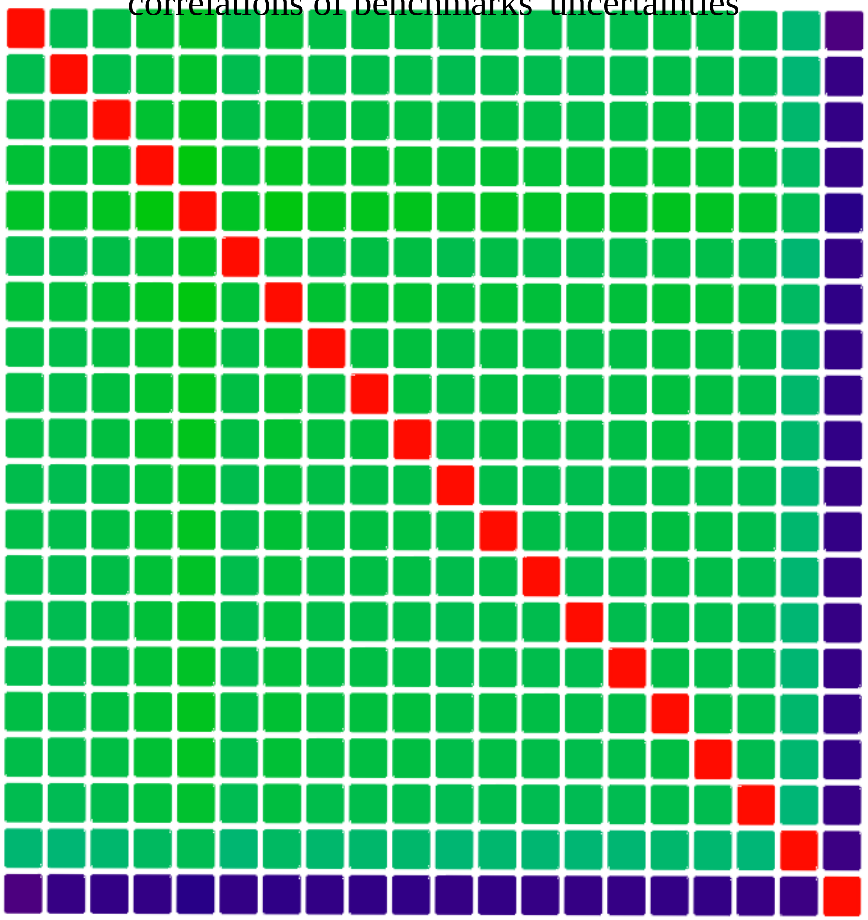
Note: sensitivity coefficients are done before normalization on number of pins

The major components of total integral experiments uncertainties (computed for this study)

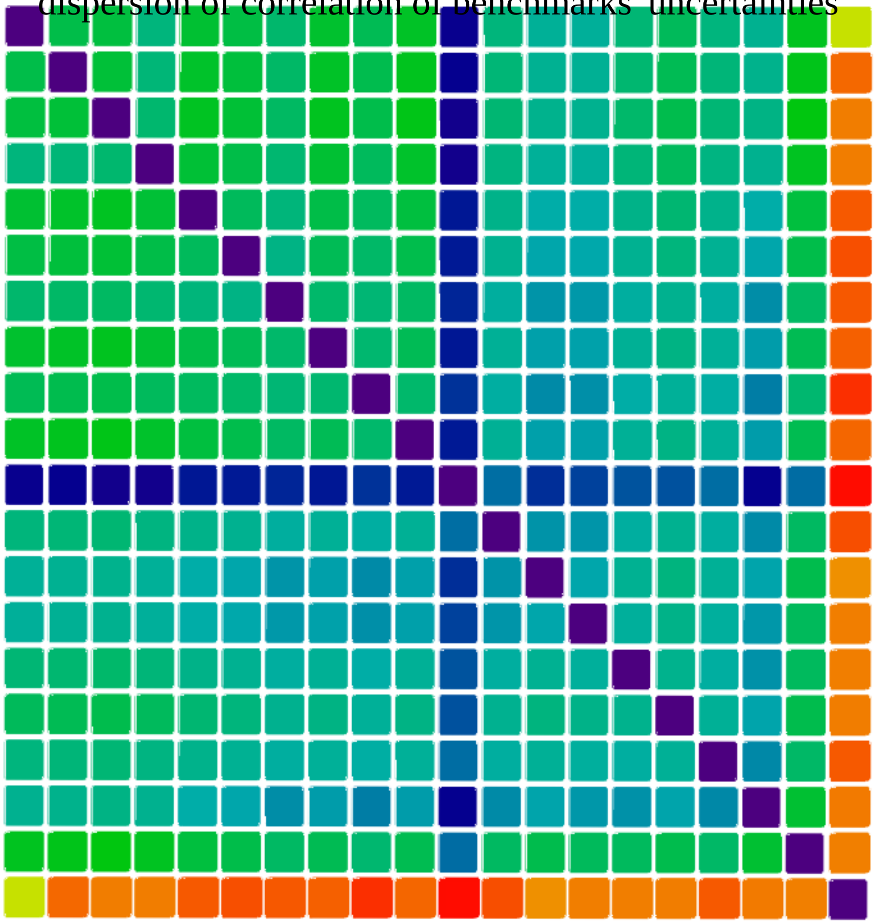
	Pin size	*Clad size*	*Mass*	*Impurities*	*Enrichment*	*Pitch*	*Critical level*
LCT-039-001	44.52	1.68	3.51	0.98	2.03	**81.57**	5.05
LCT-039-003	43.96	1.59	3.56	1.01	2.21	**79.36**	4.94
LCT-039-003	39.47	1.46	3.82	0.99	2.07	**74.53**	5.88
LCT-039-004	39.24	1.30	4.34	1.01	2.09	**78.81**	2.00
LCT-039-005	29.37	1.05	4.99	0.96	2.18	**65.11**	3.66
LCT-039-006	29.99	1.18	4.81	0.95	1.98	**59.72**	10.21
LCT-039-007	37.87	1.54	3.28	0.89	1.13	**76.20**	6.66
LCT-039-008	38.86	1.90	4.07	1.06	1.86	**74.77**	7.43
LCT-039-009	35.28	1.99	4.22	0.85	2.50	**70.04**	9.64
LCT-039-010	30.12	1.29	3.25	0.91	2.05	**62.97**	12.18
LCT-039-011	45.27	1.36	2.84	1.07	2.06	**82.04**	4.02
LCT-039-012	42.61	1.56	3.52	0.90	0.71	**79.72**	5.97
LCT-039-013	42.09	2.54	3.32	1.00	1.71	**77.52**	5.94
LCT-039-014	41.61	1.57	3.96	0.89	2.00	**76.17**	6.55
LCT-039-015	40.64	1.88	3.58	0.94	2.16	**75.18**	6.63
LCT-039-016	39.03	1.83	3.48	0.36	2.16	**74.50**	6.90
LCT-039-017	39.49	2.92	4.26	0.86	2.07	**74.64**	7.10
LCT-007-001	48.61	1.67	2.78	1.05	1.34	**86.19**	3.69
LCT-007-002	21.62	0.30	5.87	0.98	3.14	**39.24**	8.57
LCT-007-003	5.39	0.61	8.24	0.98	3.13	**-9.35**	5.15

Correlation matrix and its dispersion

correlations of benchmarks' uncertainties



dispersion of correlation of benchmarks' uncertainties

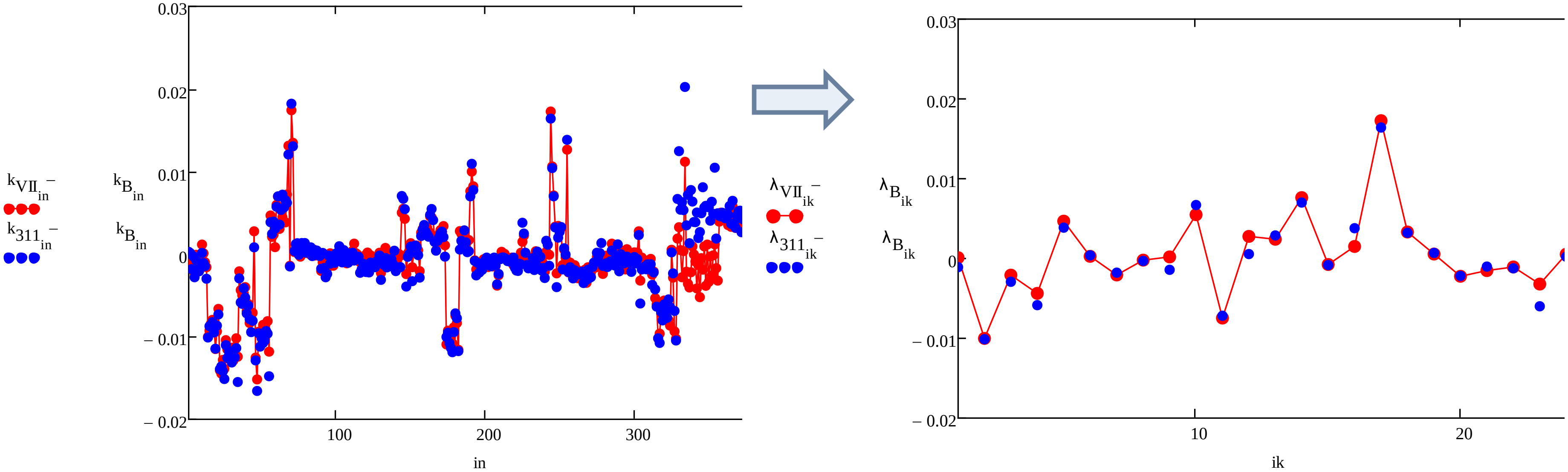


Correlation matrix of integral experiments uncertainties w/o pitch, x 1000

	Δk, pcm	LCT-039-001	LCT-039-002	LCT-039-003	LCT-039-004	LCT-039-005	LCT-039-006	LCT-039-007	LCT-039-008	LCT-039-009	LCT-039-010
LCT-039-001	**45.03**	1000.00									
LCT-039-003	**44.47**	999.99	1000.00								
LCT-039-003	**40.18**	999.22	999.24	1000.00							
LCT-039-004	**39.62**	997.56	997.72	995.26	1000.00						
LCT-039-005	**30.13**	995.59	995.89	996.92	995.56	1000.00					
LCT-039-006	**32.14**	974.59	974.61	982.55	961.80	979.69	1000.00				
LCT-039-007	**38.64**	997.99	997.85	999.35	991.90	994.45	985.71	1000.00			
LCT-039-008	**39.87**	996.78	996.74	999.06	990.47	995.44	989.22	999.55	1000.00		
LCT-039-009	**36.96**	987.30	987.29	992.58	976.87	988.52	997.34	994.50	996.71	1000.00	
LCT-039-010	**32.75**	963.43	963.29	972.48	945.67	964.81	997.15	977.59	981.10	992.97	1000.00
LCT-039-011	**45.61**	999.55	999.55	997.68	998.14	993.53	967.91	995.94	994.06	982.48	956.17
LCT-039-012	**43.22**	999.24	999.07	999.25	995.08	994.64	979.12	999.30	998.02	989.98	969.21
LCT-039-013	**42.76**	999.38	999.28	999.49	995.14	995.07	979.58	999.15	998.42	991.04	999.06
LCT-039-014	**42.40**	998.95	998.94	999.95	994.38	996.44	983.80	999.64	999.36	993.41	974.27
LCT-039-015	**41.44**	998.73	998.70	999.82	993.61	995.79	984.32	999.64	999.48	994.02	975.48
LCT-039-016	**39.90**	997.88	997.84	999.43	991.94	995.10	986.29	999.57	999.61	995.28	978.17
LCT-039-017	**40.51**	996.92	996.87	998.86	991.30	995.74	987.29	999.03	999.62	995.79	978.49
LCT-007-001	**48.89**	998.93	998.83	996.40	997.96	991.77	963.89	994.79	992.35	979.39	951.72
LCT-007-002	**24.21**	948.57	949.12	960.10	937.07	964.73	991.55	961.75	968.61	982.61	986.52
LCT-007-003	**11.60**	580.33	582.46	606.59	578.28	648.43	701.78	603.87	625.22	663.23	684.03

	Δk, pcm	LCT-039-011	LCT-039-012	LCT-039-013	LCT-039-014	LCT-039-015	LCT-039-016	LCT-039-017	LCT-007-001	LCT-007-002	LCT-007-003
LCT-039-011	**45.61**	1000.00									
LCT-039-012	**43.22**	998.11	1000.00								
LCT-039-013	**42.76**	998.12	999.44	1000.00							
LCT-039-014	**42.40**	997.22	999.31	999.47	1000.00						
LCT-039-015	**41.44**	996.92	999.06	999.56	999.91	1000.00					
LCT-039-016	**39.90**	995.71	998.51	999.05	999.67	999.81	1000.00				
LCT-039-017	**40.51**	994.23	997.73	998.77	999.07	999.34	999.41	1000.00			
LCT-007-001	**48.89**	999.74	997.64	997.33	995.93	995.54	994.15	992.68	1000.00		
LCT-007-002	**24.21**	939.63	952.56	953.82	961.19	961.42	964.04	966.20	933.24	1000.00	
LCT-007-003	**11.60**	560.08	585.36	589.89	607.29	606.15	611.07	624.50	546.76	783.16	1000.00

ND Library, figure of merit, impact of correlations



<u>**Weighted mean biases (figure of merit) for water-LEU lattices**</u>

[S. van der Marck, ND Sheets 113 (2012) 2935-3005], [this work]

	ENDF/B-VII.1	JEFF-3.1.1
LCT long list	-20.8	11.8
LCT correlated set	54.4	138.9

Conclusions

Action 1

- The uncertainties and correlations of the integral benchmarks of ICSBEP Handbook have been evaluated with "uncertainties-of-uncertainties"
- The selected cases have been found to be almost entirely correlated

- The 2-nd sections in ICSBEP benchmarks profiles provide enough data for experimental uncertainties correlations establishment
- Correlations being applied change the evaluated accuracy levels of ND libraries

Action 2

- "Equivalence theory" being applied to ^{235}U bare spherical experimental configurations demonstrates contradictions

Action 3 (TBD to ensure consistency of the integral experimental data)

- elaborate uncertainties and their correlations in the "integral field"
- work on PFNS for U and Pu (if possible), and on ZPR-6 issues

Thank you for your attention.

Questions?