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KIT contribution to UAM PHASE-I: modellig and updated results

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UAM-9 Workshop, Madrid (Spain), 20-22.05.2015

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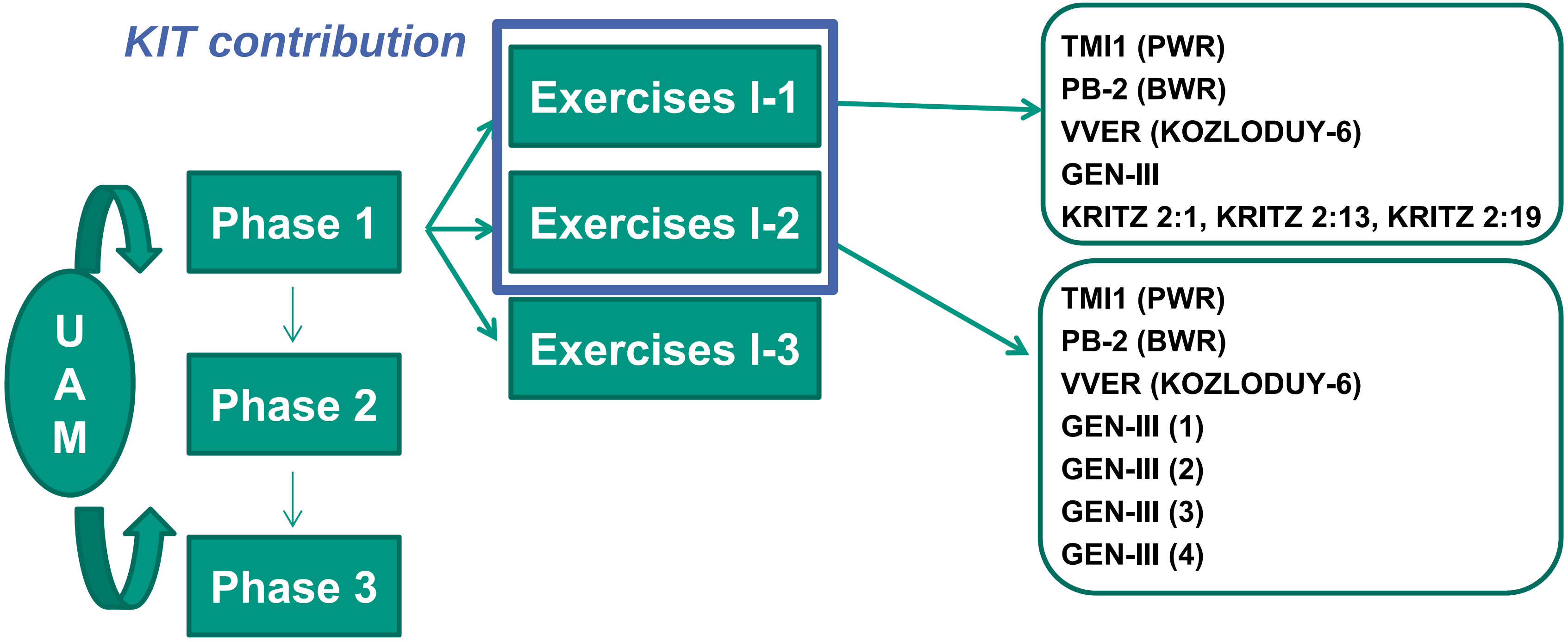
Introduction

KIT-INR/RPD contribution to the UAM neutronics exercises:

- **Monte Carlo** (reference) solutions ⟶ **SERPENT 1.18** code
- **Deterministic** solutions ⟶ **SCALE** code (6.1 and 6.2b3)



Computational methodologies

- **SERPENT code (version 1.1.18)**
  - Different NDLs: JEFF3.1, JEFF3.1.1, ENDF/B-VII
  - Statistics: 5.0e+06 neutrons sources over 1000 cycles

- **SCALE code (version 6.1)**
  - ENDF/B-VII
  - Transport (NEWT, XSDRNPM)
  - S/U analysis via perturbation theory: TSUNAMI

$$Q = f(\sigma_1, \sigma_2, \ldots, \sigma_n)$$ **Integral parameter**

$$\frac{\delta Q}{Q} = \sum_j S_j \frac{\delta \sigma_j}{\sigma_j} \Longrightarrow S_j = \frac{\partial Q}{\partial \sigma_j} \cdot \frac{\sigma_j}{Q}$$ **Sensitivity coefficient**

$$var(Q) = \sum_{j,i}^{J} S_j S_i d_{ij}$$ **Uncertainty**

$$D_\sigma = \begin{bmatrix} d_{11} & \cdots & d_{1J} \\ \vdots & \ddots & \vdots \\ d_{1J} & \cdots & d_{JJ} \end{bmatrix}$$ **Covariance matrix**

Monte-Carlo (reference) solutions

Test cases I-1		Kinf		
		JEFF3.1	JEFF 3.1.1	ENDFB-7
VVER	HZP	1.34764 ± 0.00028	1.34937 ± 0.00026	1.34986 ± 0.00027
	HFP	1.33152 ± 0.00028	1.33356 ± 0.00029	1.33435 ± 0.00029
PWR	HZP	1.42785 ± 0.00027	1.42888 ± 0.00025	1.42923 ± 0.00027
	HFP	1.41136 ± 0.00026	1.41315 ± 0.00028	1.41401 ± 0.00026
BWR	HZP	1.34541 ± 0.00027	1.34673 ± 0.00025	1.34691 ± 0.00026
	HFP	1.23046 ± 0.00032	1.23080 ± 0.00032	1.23295 ± 0.00032
KRITZ-2:1	Cold	1.23762 ± 0.00028	1.23846 ± 0.00027	1.23984 ± 0.00027
	Hot	1.22632 ± 0.00028	1.22864 ± 0.00026	1.22863 ± 0.00027
GEN-III	HFP	1.01485 ± 0.00039	1.01602 ± 0.00039	1.01805 ± 0.00037

Test cases I-2		Kinf		
		JEFF3.1	JEFF 3.1.1	ENDFB-7
PWR	HZP	1.41569 ± 0.00019	1.41733 ± 0.00019	1.41839 ± 0.00019
	HFP	1.40616 ± 0.00020	1.40765 ± 0.00019	1.40852 ± 0.00018
BWR	HZP	1.11771 ± 0.00025	1.11830 ± 0.00025	1.11913 ± 0.00025
	HFP	1.07503 ± 0.00028	1.07663 ± 0.00029	1.07739 ± 0.00027
GEN-III type 1 (UOX 2.1%)		1.04854 ± 0.00022	1.05043 ± 0.00021	1.05159 ± 0.00022
GEN-III type 1 (UOX 4.2%)		1.25708 ± 0.00019	1.25951 ± 0.00019	1.25997 ± 0.00020
GEN-III type 2		1.12760 ± 0.00027	1.12937 ± 0.00026	1.13048 ± 0.00026
GEN-III type 3		1.05005 ± 0.00030	1.05148 ± 0.00029	1.13048 ± 0.00026
GEN-III type 4		1.11595 ± 0.00025	1.11706 ± 0.00025	1.11697 ± 0.00025

Good agreement within different data libraires and with previous MCNP (PSU) results

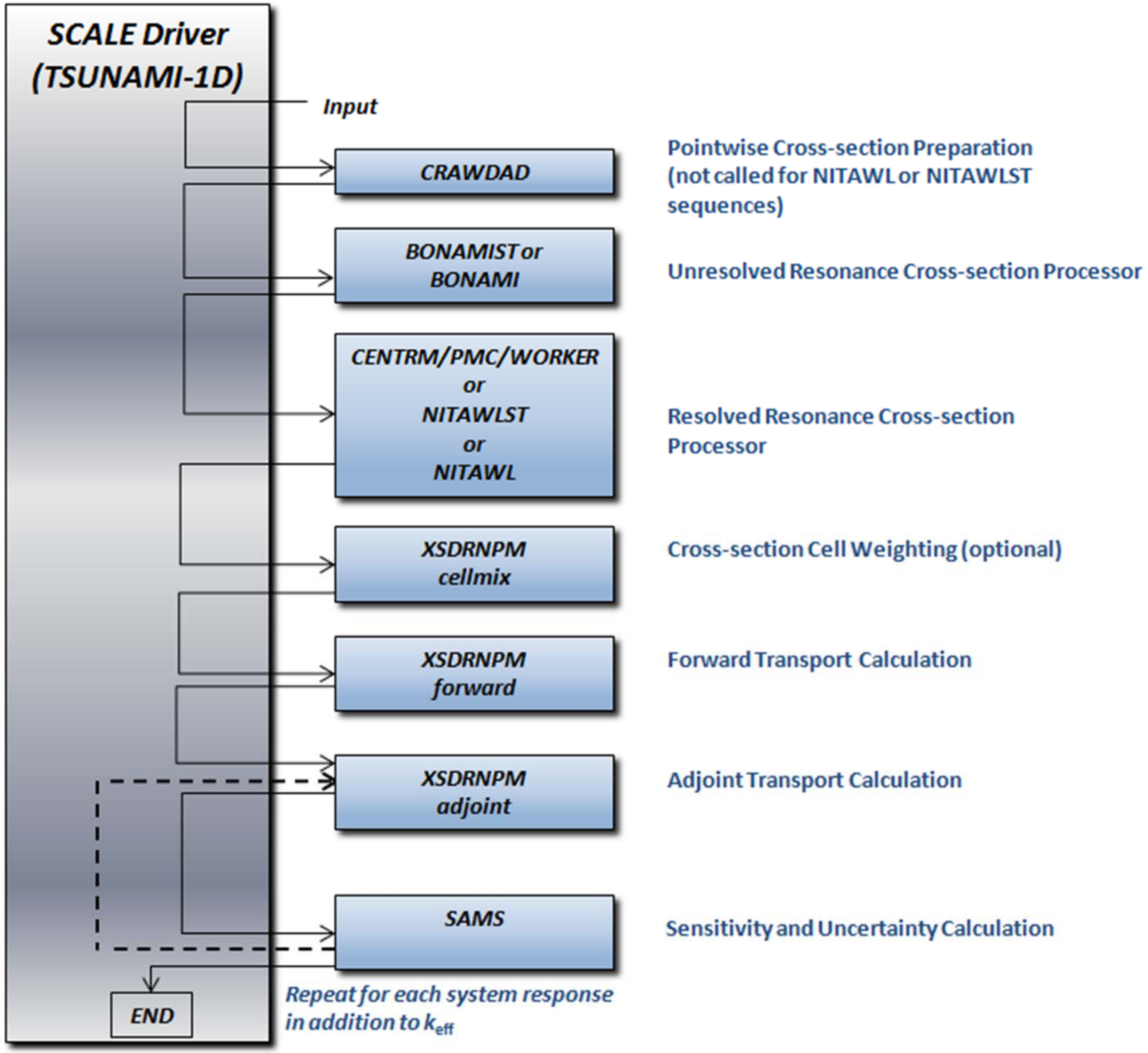
Computational method: TSUNAMI-1d flow diagram

ENDF/B-VII.0

Transport
Discrete Ord.
238-groups

Sensitivities
via GPT

44GROUPCV



Exercises I-1: Cell Physics

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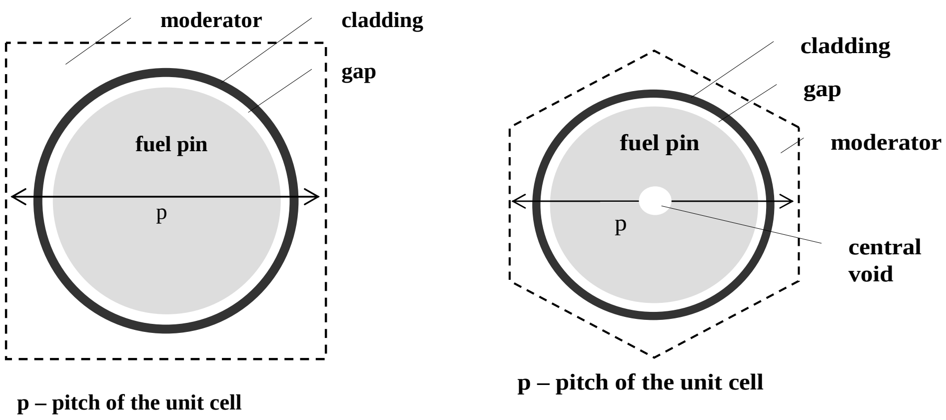
Focuses on the derivation of the multi-group microscopic cross section libraries (in the way used as inputs by the lattice physics codes) and their uncertainties

<u>Test cases</u>:

- PB-2 (BWR)
- TMI1 (PWR)
- GEN-III (MOX fuel)
- KRITZ 21, KRITZ 213, KRITZ 219
- VVER (KOZLODUY-6)



Exercise I-1: k-inf

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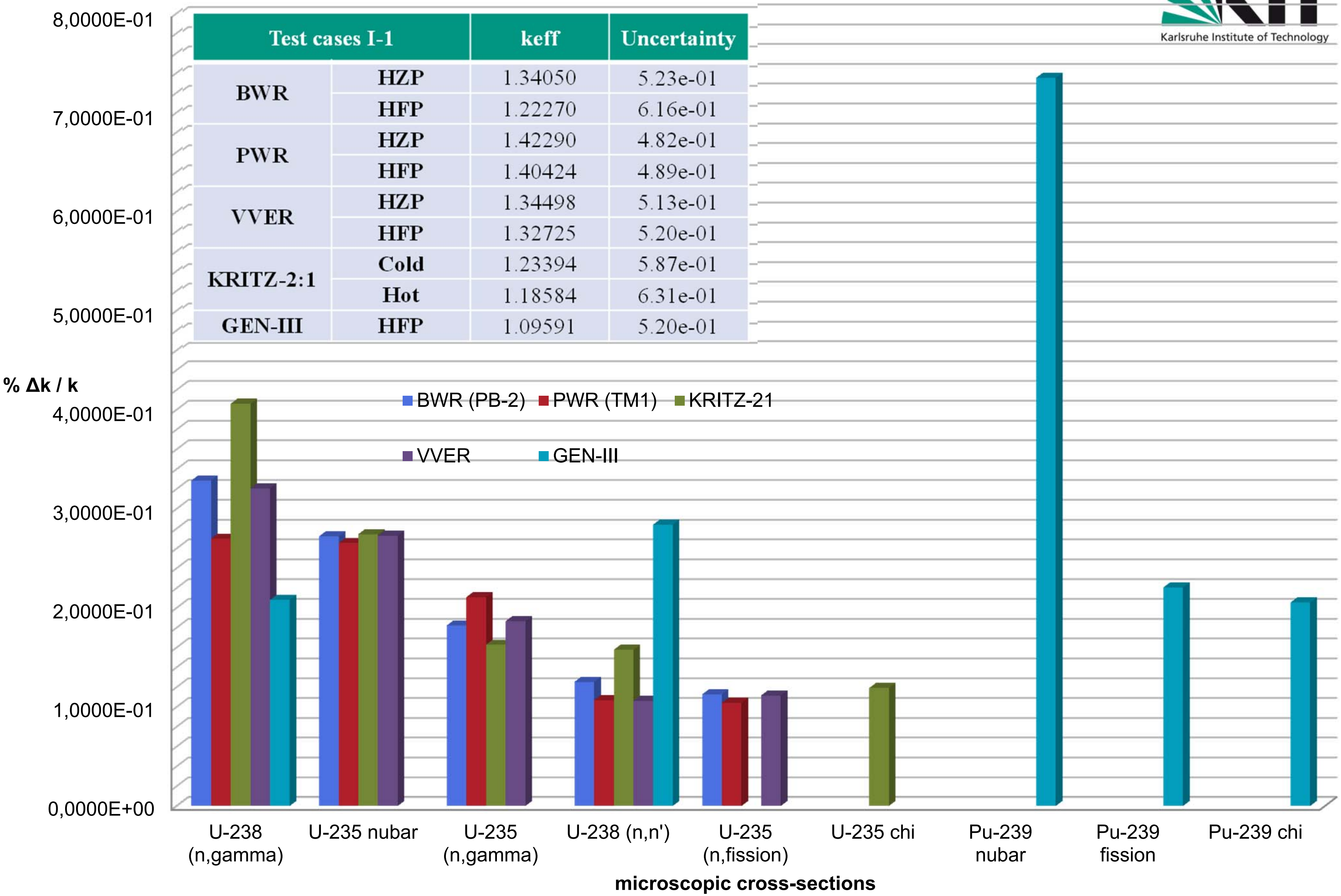
Test cases I-1		keff	Uncertainty
BWR	HZP	1.34050	5.23e-01
	HFP	1.22270	6.16e-01
PWR	HZP	1.42290	4.82e-01
	HFP	1.40424	4.89e-01
VVER	HZP	1.34498	5.13e-01
	HFP	1.32725	5.20e-01
KRITZ-2:1	Cold	1.23394	5.87e-01
	Hot	1.18584	6.31e-01
GEN-III	HFP	1.09591	5.20e-01



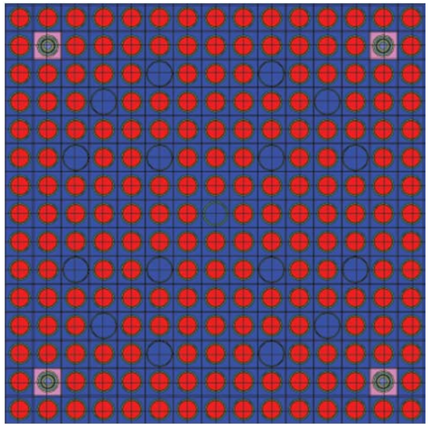
SCALE vs. SERPENT

Micro-XS	SCALE 6.1 [barns]	SERPENT [barns]	Uncertainty (%)	Unit cell
U-235 abs.	41.48	40.41 ± 0.0086	1.22	BWR
U-238 abs.	0.88	0.80 ± 0.0011	0.97	
U-235 fission	33.43	32.56 ± 0.00069	1.22	
U-238 fission	0.086	0.089 ± 0.00097	4.79	
U-235 abs.	42.95	42.18 ± 0.00088	1.09	PWR
U-238 abs.	0.96	0.93 ± 0.0011	0.97	
U-235 fission	34.72	34.10 ± 0.00064	1.11	
U-238 fission	0.099	0.10 ± 0.00096	3.94	
U-235 abs.	58.13	57.26 ± 0.00085	1.03	VVER
U-238 abs.	1.042	1.005 ± 0.0012	0.99	
U-235 fission	47.84	47.76 ± 0.00063	1.05	
U-238 fission	0.093	0.095 ± 0.00100	3.88	

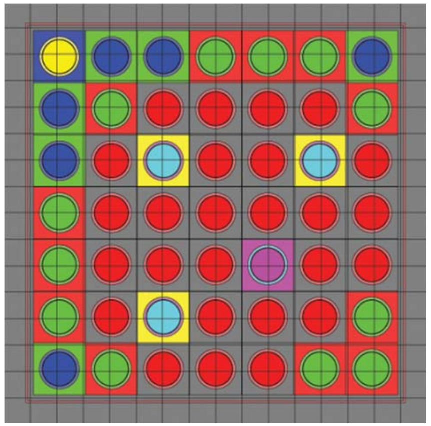
Uncertainties on micro-XSs higher by an order of magnitude with respect to those on K_{eff}

Exercises I-2: Lattice Physics

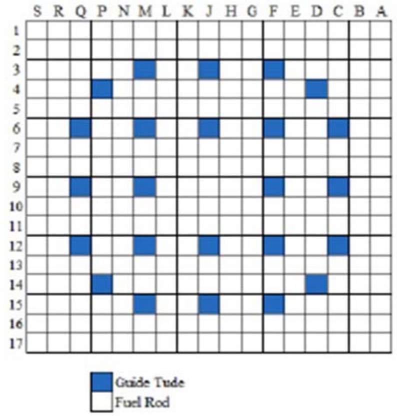
Multigroup cross-section uncertainties from Exercise I-1 are propagated through lattice physics calculations to 2 groups (Ecutoff = 0.625 eV) microscopic uncertainties



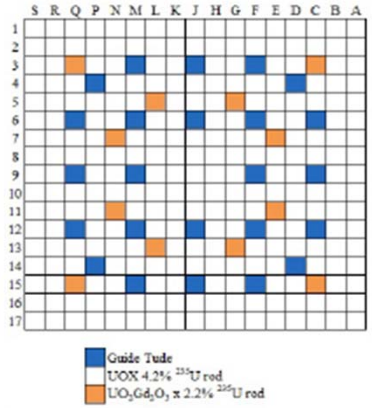
PWR



BWR

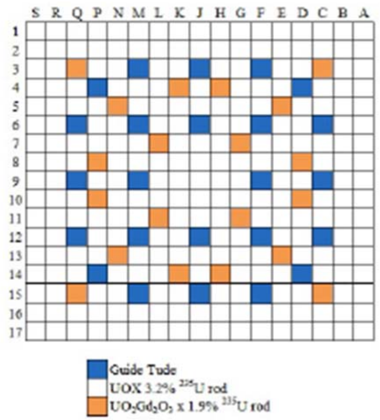


Type 1: UOX 2.1% ^{235}U without UO_2-Gd_2O_3 rods UOX 4.2% ^{235}U assembly without UO_2-Gd_2O_3 rods

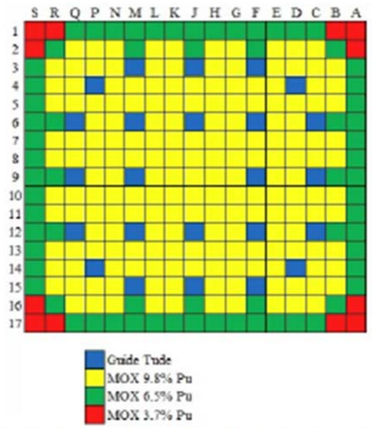


Type 2: UOX 4.2% ^{235}U assembly with 12 UO_2 Gd_2O_3 (2.2% ^{235}U) rods

GEN-III



Type 3: UOX 3.2% ^{235}U assembly with 20 UO_2-Gd_2O_3 (1.9% ^{235}U) rods



Type 4: MOX assembly (without UO_2-Gd_2O_3 rods)

Exercises I-2: results

Test Case		k-eff	Uncertainty
BWR	HZP	1.11029	5.00E-01
	HFP	1.07736	5.56E-01
PWR	HZP	1.41009	4.64E-01
	HFP	1.39351	4.71E-01
GEN-III (1)	HFP	1.25325	4.87E-01
GEN-III (2)	HFP	1.12304	4.94E-01
GEN-III (3)	HFP	1.04501	5.03E-01
GEN-III (4)	HFP	1.07008	9.68E-01

Keff Sensitivities			Keff Uncertainties		
XS	BWR	PWR	XS	BWR	PWR
U-235 nubar	9.19E-1	9.45E-1	U-238 (n,γ)	3.20E-1	2.56E-1
U-235 fission	4.15E-1	2.73E-1	U-235 nubar	2.65E-1	2.68E-1
U-235 total	3.08E-1	1.25E-1	U-238 (n,n')	2.06E-1	9.72E-2
H-1 elastic	1.66E-1	1.66E-1	U-235 chi	1.47E-1	8.79E-2
H-1 scatter	1.65E-1	1.66E-1	U-235 (n,γ)	1.44E-1	2.00E-1

Exercises I-2: homogenized XS uncertainties

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Cross-section	Energy group	Value (cm^{-1}) (Uncertainty %) PWR	BWR	GEN-III Type 1	GEN-III Type 2	GEN-III Type 3	GEN-III Type 4
Total	1	1.44E + 00 (1.38E – 01)	1.58E + 00 (1.29E – 01)	1.31E + 00 (1.41E – 01)	1.32E + 00 (1.39E – 01)	1.33E + 00 (1.39E – 01)	1.50E + 00 (1.39E – 01)
	2	5.69E – 01 (8.78E – 01)	5.79E – 01 (8.40E – 01)	5.33E – 01 (9.04E – 01)	5.34E – 01 (9.03E – 01)	5.34E – 01 (9.01E – 01)	5.24E – 01 (9.73E – 01)
Absorption	1	1.11E – 01 (8.77E – 01)	5.72E – 02 (6.06E – 01)	1.07E – 01 (7.00E – 01)	1.17E – 01 (5.61E – 01)	3.45E – 1 (9.79E – 01)	1.24E – 01 (5.11E – 01)
	2	1.06E – 02 (1.33E + 00)	7.32E – 03 (1.38E + 00)	1.04E – 02 (1.35E + 00)	1.06E – 02 (1.34E + 00)	5.09E – 01 (1.47E + 00)	1.07E – 02 (1.34E + 00)
Fission	1	7.95E – 01 (3.17E – 03)	2.94E – 02 (3.23E – 01)	6.86E – 02 (3.23E – 01)	6.60E – 02 (3.24E – 01)	1.90E – 01 (6.26E – 01)	6.42E – 02 (3.24E – 01)
	2	3.59E – 03 (3.55E – 01)	1.95E – 03 (6.81E – 01)	3.17E – 03 (3.71E – 01)	3.10E – 03 (3.75E – 01)	4.97E – 01 (4.45E – 01)	3.05E – 03 (3.80E – 01)
Nufission	1	1.94E – 01 (4.44E – 01)	7.02E – 02 (4.49E – 01)	1.67E – 1 (4.48E – 01)	1.61E – 01 (4.49E – 01)	5.45E – 01 (1.09E + 00)	1.56E – 01 (4.49E – 01)
	2	9.08E – 03 (5.12E – 01)	4.69E – 03 (1.01E + 00)	8.02E – 03 (5.71E – 01)	7.86E – 03 (5.82E – 01)	1.44E – 02 (7.75E – 01)	7.73E – 3 (5.92E – 01)

The GRS Method (1)

- The Wilk's formula is used to determine the number of calculations required to obtain the uncertainty bands.
- The number of code runs is independent of the number of selected input uncertainty parameters

$$1-\alpha^{n} \geq \beta$$ (One sided)

$$1-\alpha^{n}-n\cdot(1-\alpha)\cdot\alpha^{n-1} \geq \beta$$ (Two sided)

α = probability content
β = confidence level that the maximum obtained code result will not be exceeded with a probability α
n = number of code runs

	One-sided statistical limits			Two-sided statistical limits		
β / α	**0.90**	**0.95**	**0.99**	**0.90**	**0.95**	**0.99**
0.90	22	45	230	38	77	388
0.95	29	59	299	46	**93**	473
0.99	44	90	459	64	130	**662**

The GRS method (2)

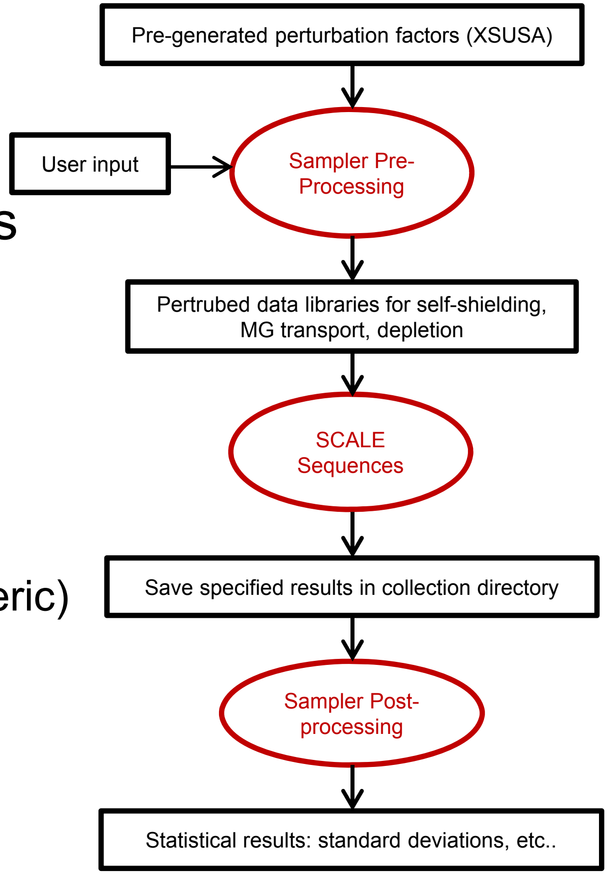
- Uncertainty in input values described by PDFs
- The model output is a random variable whose distribution reflects the uncertainty in the output associated with the uncertainty in the input
- The objective of the uncertainty analysis is to obtain information about the probability distribution of the output
- One would like to know exactly the probability distribution of the output in order to answer as precise as possible all questions about the likelihood of its values
- Unfortunately the distribution cannot be derived analytically and the assumption of normal distribution is made
- Statististics offers the means to “quantify” the goodness of our output values (Chi-Square normality test, etc.)

SCALE/*Sampler* at KIT

- Extensive assessment of SCALE/Sampler at KIT in 2014

- *Sampler* is a SCALE "super-sequence"

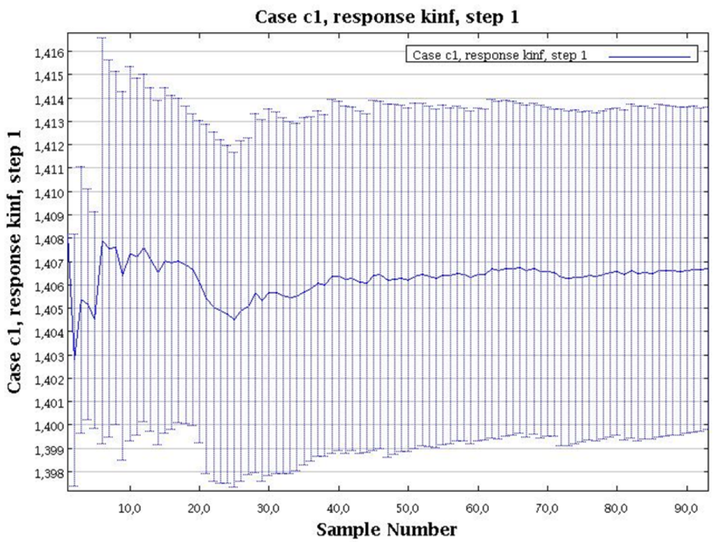
- Sampling results for following types of responses
  - K eingenvalue (XSDRN, NEWT, KENO)
  - Microscopic reaction rates by nuclide (Newt/Opus)
  - Homogenized/collapsed macro cross sections (Newt)
  - Nuclide concentrations, activities (ORIGEN)
  - Decay heat, radiotoxicity, photon sources (ORIGEN)
  - Schield responses: doses, radiation damage, etc. (Maveric)

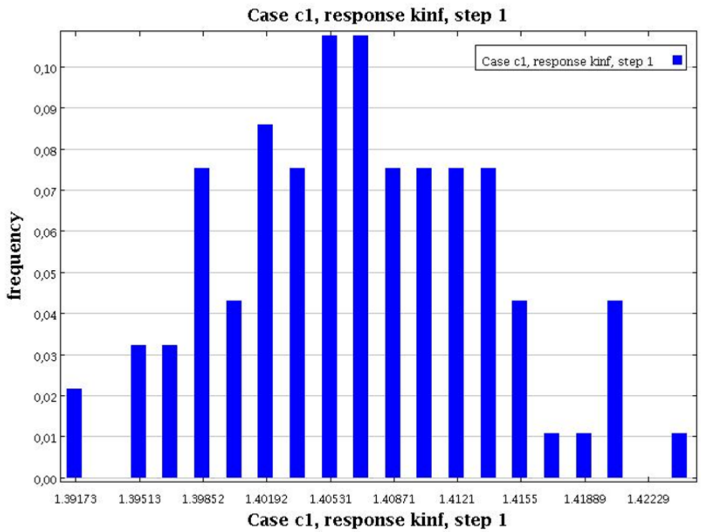


- Each response at every time-step includes:
  - Frequency distributions as histogram plot file
  - Mean values and standard deviations in CSV file
  - Results of chi-squared normality test for each response
  - Covariance and correlation coefficients between responses

LWRs-pin cells: sampling approach vs. perturbation theory

HZP	TSUNAMI		SAMPLER (N=93)	
	k	% δk/k	k	% δk/k
BWR (HFP)	1.22270	6.16E-01	1.22533	6.23E-01
BWR (HZP)	1.34050	5.23E-01	1.34249	5.18E-01
PWR (HZP)	1.42290	4.89E-01	1.40670	4.88E-01
PWR (HFP)	1.40424	4.82E0-1	1.42635	4.79E-01
VVER (HFP)	1.32725	5.20E-01	1.32993	5.12E-01
VVER (HZP)	1.34498	5.13E-01	1.34879	5.04E-01
VVER - 1000	0.36112	1.24E+00		1.36E+00





PWR (HFP)

VVER Fuel Assembly (Kozloduy - 6)

Test cases	TSUNAMI	Uncertainty [%]	SAMPLER	Uncertainty [%]
VVER-1000				
HZP_{rodded}	0.94730	5.08E-01	0.94591	5.04E-01
HFP_{rodded}	0.93199	5.12E-01	0.93328	5.12E-01
$HZP_{unrodded}$	1.33818	5.03E-01	1.34050	4.83E-01
$HFP_{unrodded}$	1.32299	5.15E-01	1.32741	4.88E-01

Reaction	Energy gr.	TSUNAMI [cm^{-1}]	SAMPLER [cm^{-1}]
Total	1	5.51E-01 (-)	5.50E-01 (8.95E-01)
	2	1.37E+00 (-)	1.37E+00 (1.50E-01)
Fission	1	2.41E-03 (5.07E-01)	2.43E-03 (5.50E-01)
	2	5.61E-02 (3.28E-01)	5.70E-02 (3.37E-01)
Absorption	1	1.41E-02 (1.34E+00)	1.41E-02 (9.08E-01)
	2	9.48E-02 (8.81E-01)	9.65E-02 (1.99E-01)
Scattering	1	5.37E-01 (8.43E-01)	5.36E-01 (8.99E-01)
	2	1.27E+00 (1.59E-01)	1.27E+00 (1.61E-01)
Nufission	1	6.16E-03 (-)	6.22E-03 (8.42E-01)
	2	1.37E-01 (-)	1.39E-01 (4.54E-01)

Good agreement between the two approaches

Summary

- The complete set of updated results for Exercises I-1 and I-2 has been provided to the benchmark team according to the new template specifications
- Uncertainties in the order of ~0.5% (k_{eff}) and ~4% (XSs)
- U-238 (n,ɣ) and Pu-239 nubar major contributors to the uncertainties for UOX and MOX LWR's test cases
- Good agreement with the Monte-Carlo solutions, especially for microscopic XSs
- Perturbation theory approach and the statistical sampling methodology provide consistent results
- Work in progress:
  - Validation of the statistical sampling methodology (SCALE 6.2b4)
  - Exercise I-3 test cases
  - Pin-cell burn-up test case I-1