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Uncertainty Quantification Using SCALE 6.2 And GPT Techniques Implemented In Serpent

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Abstract – *The use of Monte Carlo codes for sensitivity and uncertainty analysis has significantly increased in recent years, in order to overcome some of the limitations of the deterministic codes. The main purpose of this work is to show the capabilities of the Monte Carlo code Serpent in sensitivity and uncertainty analysis, comparing Serpent results with SCALE 6.1 and 6.2. Moreover, the new 56 groups covariance library available in SCALE 6.2 is tested. This work is done in the framework of the OECD/NEA benchmark for Uncertainty Analysis in Modeling. The test case under consideration is the Three Mile Island Pressurized Water Reactor fuel pin in Hot Zero Power conditions. It was found a good agreement between SCALE and Serpent sensitivity calculations. The differences found between the covariance libraries used are highlighted.*

I. INTRODUCTION

In recent years there has been an increasing demand from nuclear research, industry, safety and regulation for best estimate predictions to be provided with their confidence bounds. Uncertainty quantification is important in order to introduce appropriate design margins and decide where additional efforts should be undertaken to reduce such uncertainties. In this framework it was decided to define an OECD benchmark for Uncertainty Analysis in Modeling (UAM) for design, operation and safety analysis of Light Water Reactors (LWR) [1].

This paper is focused on exercise I of the first phase of the UAM benchmark [2]. In particular, the TMI PWR fuel pin in HZP conditions is chosen as test case. As requested by the benchmark, uncertainty with its top contributors is calculated for several response functions: k_{eff} and one-group microscopic capture and fission cross sections of ^{235}U and ^{238}U.

Such uncertainties are calculated in two different ways, using Monte Carlo code Serpent and SCALE suite. SCALE is a well-established tool that allows sensitivity and uncertainty calculation for LWR analysis. Serpent is a 3D continuous energy Monte Carlo reactor physics code and a modified version of the code with implemented Generalized Perturbation Theory (GPT) techniques was recently developed [3]. The development of methods for sensitivity/perturbation calculations with Monte Carlo codes is of big interest for the international R&D community, in order to overcome some of the limitations of the deterministic codes. This aspect is evidenced by the large efforts spent during the recent years in this field [4-7].

One of the objectives of this work is to provide a validation of the Serpent-GPT code against SCALE 6.1 and 6.2 [8], demonstrating the applicability of the Serpent code for sensitivity and uncertainty analysis. Another of the purposes of the work is to compare uncertainty quantification with different covariance matrices, in particular with the new 56 group covariance matrix of SCALE 6.2 [8].

The paper is structured as follows. Section 2 gives an overview of the methods and codes used for the calculation. Section 3 contains the description and specifications of the test case. Section 4 presents the results of the SCALE and Serpent calculation. Section 5 summarizes the paper and draws conclusions.

II. METHODS AND CODES

This section gives a brief overview of the methods and codes used for the analysis.

1. Serpent-GPT

Serpent is a 3D continuous energy Monte Carlo reactor physics burnup calculation code, developed at VTT Technical Research Centre of Finland [9]. In this work, version 2.1.22 of Serpent is used. This code has been modified in order to implement GPT techniques for sensitivity and uncertainty analysis. The developed methods are based on the concepts of ‘‘rejected event’’ and ‘‘collision history’’. The considered perturbed parameters x can be regarded as probability distributions for given events (e.g., the occurrence of a collision, the emission of a neutron with a given outgoing energy, the sampling of a scattering cosine, etc.). Probability density functions for the considered events are biased and the sampling process is artificially altered. To restore ‘‘fair’’ neutron transport, sampled events are rejected according to the introduced biases. Both real (accepted) and virtual (rejected) events are recorded and form the collision history of each particle. This collision history, passed to neutron descendants, is adopted to compute the effects of a perturbation of a parameter x on the considered response functions R [3]. The sensitivity coefficient $S_{R,x}$ is defined as:

$$S_{R,x} = \frac{dR/R}{dx/x} \tag{1}$$

Once the sensitivity coefficients are calculated for the desired response functions (e.g. k_{eff} and microscopic cross sections), uncertainty is obtained using the sandwich rule:

$$Var[R] = S_{R,x} Cov[x] (S_{R,x})^T \tag{2}$$

Where Cov[x] is the covariance matrix of x. Uncertainty is here expressed as standard deviation σ:

$$\sigma[R] = \sqrt{Var[R]} \tag{3}$$

2. SCALE – TSUNAMI 1D

The SCALE Code System is a widely-used modeling and simulation suite for nuclear safety analysis and design that is developed, maintained, tested, and managed by the Reactor and Nuclear Systems Division of Oak Ridge National Laboratory [8]. TSUNAMI-1D (Tools for Sensitivity and Uncertainty Analysis Methodology Implementation in One Dimension) is a SCALE control module that facilitates the application of sensitivity and uncertainty analysis theory to nuclear systems analyses [10, 11]. Different functional modules are executed with TSUNAMI-1D, as shown in Fig. 1.

By default, the TSUNAMI-1D sequence performs cross-section processing with XSProc. Then, the XSDRNPM module is used as transport solver, performing two criticality calculations, one forward one adjoint. XSDRNPM uses the method of discrete ordinates. The BONAMIST code computes the sensitivity of resonance self-shielded cross to the input data, the so-called "implicit sensitivities". Finally, the sequence calls the SAMS module to calculate the sensitivity coefficients and the uncertainty in the calculated value due to uncertainties in the basic nuclear data. Versions 6.2 and 6.1 of SCALE are used in this work.

3. Covariance matrices

One of the purposes of this study is to compare uncertainty quantification with different covariance matrices. Therefore, the following covariance data libraries are used in the calculation:

- 44-group from SCALE 6.1
- 56-group from SCALE 6.2

The isotopes considered in the uncertainty quantification are:

- 238U
- 235U
- 16O
- 1H

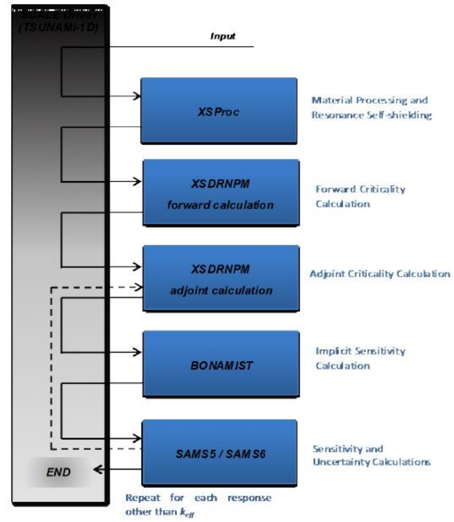

Fig. 1. General flow diagram of TSUNAMI-1D [8]

while the perturbed reactions are:

- (n, elastic)
- (n, n')
- (n, fission)
- (n, γ)
- nubar
- χ

Results with the different covariance libraries are presented and discussed in section IV.

III. DESCRIPTION OF THE TEST CASE

Both Serpent and SCALE calculations are applied to the TMI PWR fuel pin model from the exercise I-1 of the OECD/NEA UAM benchmark. The case consists of a single UO2 fuel pin, 4.85% enriched in ^{235}U, modeled in HZP conditions. The test case specifications are shown in Table I.

Table I. TMI Fuel Pin HZP Specifications

Parameter	Value
Unit cell pitch, mm	14.427
Fuel pellet diameter, mm	9.391
Fuel pellet material	UO_2
Fuel density, g/cm^3	10.283
Fuel temperature, K	551
Fuel enrichment, w %	4.85
Cladding outside diameter, mm	10.928
Cladding thickness, mm	0.673
Cladding material	Zircaloy-4
Cladding density, g/cm^3	6.55
Cladding temperature, K	551
Gap material	Helium
Moderator material	H_2O
Moderator density, g/cm^3	0.766
Moderator temperature, K	551

IV. RESULTS

In this section the results obtained in the Serpent-GPT and SCALE calculations are presented and discussed.

1. k_{eff} Uncertainty

The sensitivity coefficients per unit lethargy of the keff to the uncertainty main contributors are shown in Fig. 2-7.

Serpent-GPT results show to be in good agreement with both SCALE 6.1 and 6.2 calculations. The relative errors between the integral values in the three calculations are below 0.75% for the majority of the reactions, except for:

- ^{238}U (n, n'): the differences between Serpent-GPT and SCALE 6.1 and 6.2 are approximately 1% and 2% respectively. It should be noted that the statistic for this reaction is more difficult than for other and probably more neutron histories are needed to improve the results.
- ^{238}U (n, γ): the differences between Serpent-GPT and SCALE 6.1 and 6.2 are approximately 5%. The biggest discrepancies in the sensitivity coefficients are between 5 eV and 500 eV, in correspondence of the ^{238}U resonances. The reason of these difference is probably due to the treatment of implicit effects of SCALE. Further investigations and analysis are necessary. Moreover, SCALE 6.2 sensitivity coefficient looks different compared to SCALE 6.1 and Serpent calculations. This is mainly due to the different group structures close to the ^{238}U resonances.

Table II shows the total uncertainty in k_{eff} in the three calculations. Table III shows the main contributors to k_{eff} uncertainty in the three calculations. SCALE 6.1 and Serpent results are in very good agreement. By contrast, SCALE 6.2 results exhibit some differences, in particular for ^{235}U nubar, ^{235}U χ and ^{1}H (n,el). Considering that SCALE 6.2 sensitivity coefficients for these reactions are in agreement with SCALE 6.1 and Serpent ones, the reason of

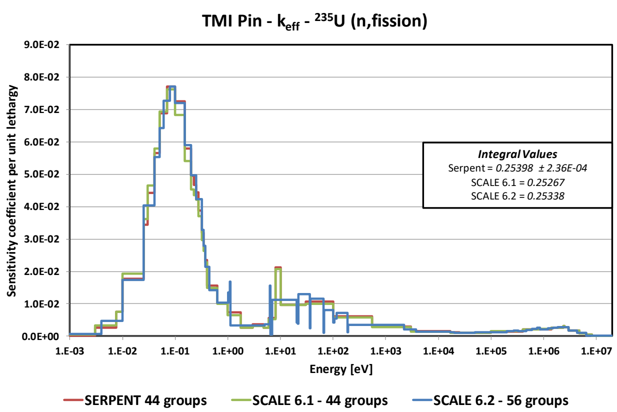

Fig. 2. Sensitivity coefficient per unit lethargy of keff to ^{235}U (n, fiss)

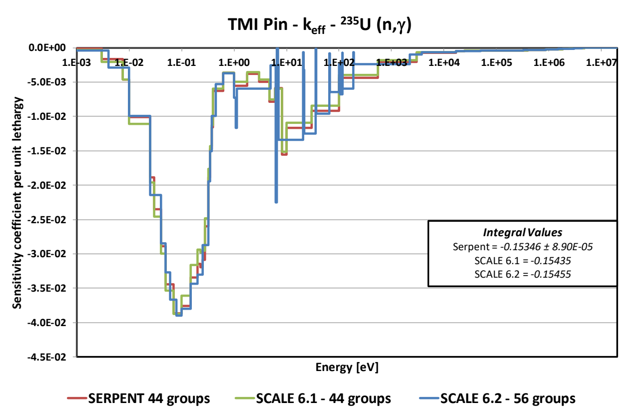

Fig. 3. Sensitivity coefficient of keff to ^{235}U (n, γ)

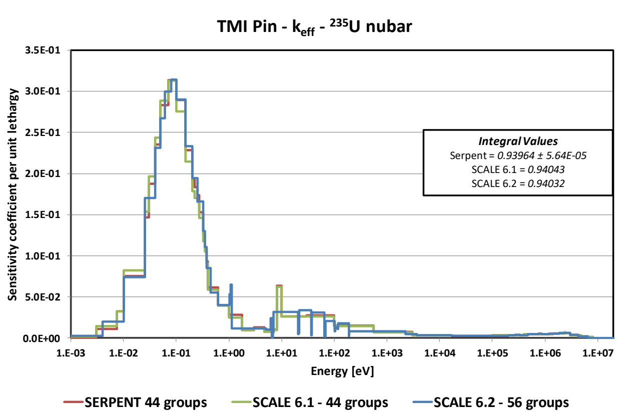

Fig. 4. Sensitivity coefficient of keff to ^{235}U nubar

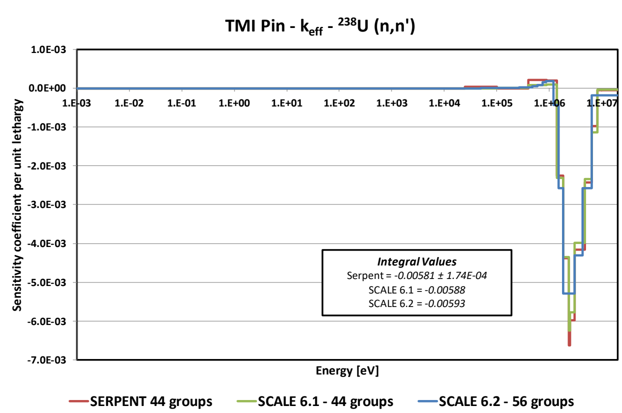

Fig. 5. Sensitivity coefficient per unit lethargy of keff to ^{238}U (n, n')

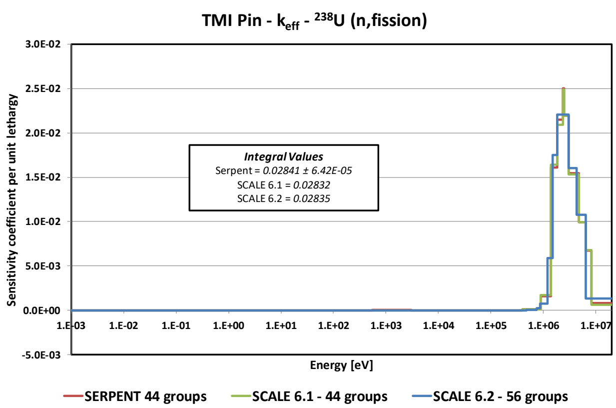

Fig. 6. Sensitivity coefficient of keff to ^{238}U (n, fiss)

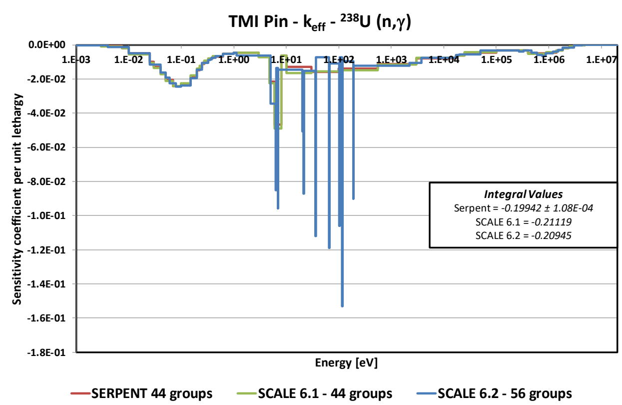

Fig. 7. Sensitivity coefficient of keff to ^{238}U (n, γ)

Table II. Total Uncertainty on k_{eff}

Serpent 44 groups		SCALE 6.1 44 groups		SCALE 6.2 56 groups	
k_{eff}	% Δk/k	k_{eff}	% Δk/k	k_{eff}	% Δk/k
1.43018 ± 4E-05	0.47%	1.42394	0.48%	1.42441	0.54%

Table III. Main contributors to k_{eff} uncertainty

Covariance Matrix		Serpent 44 groups Relative standard deviation in k_{eff} (pcm)	SCALE 6.1 44 groups Relative standard deviation in k_{eff} (pcm)	SCALE 6.2 56 groups Relative standard deviation in k_{eff} (pcm)
^{235}U nubar	^{235}U nubar	264.63	264.78	341.22
^{238}U (n,γ)	^{238}U (n,γ)	253.32	269.32	275.11
^{235}U (n,γ)	^{235}U (n,γ)	208.99	210.53	196.52
^{238}U (n,n')	^{238}U (n,n')	114.25	113.08	113.6
^{235}U χ	^{235}U χ	93.73	92.72	152.32
^{235}U (n,fiss)	^{235}U (n,fiss)	76.86	76.26	76.65
^{238}U nubar	^{238}U nubar	70.47	69.66	70.41
^{1}H (n,el)	^{1}H (n,el)	23.97	24.9	16.15

these differences are due to the new 56 groups covariance matrices of SCALE 6.2. The new covariance data files show that:

- uncertainty in ^{235}U nubar is approximately 30% higher than in the 44 groups covariances.
- uncertainty in ^{235}U χ is approximately 65% higher than in the 44 groups covariances.
- uncertainty in ^{1}H (n,el) is approximately 35% lower than in the 44 groups covariances.

2. One-group σ Uncertainty

In order to calculate the uncertainty of one-group microscopic capture and fission cross sections of ^{235}U and ^{238}U, the sensitivity coefficients to the uncertainty main contributors have to be evaluated. In this case it should be noted that sensitivity coefficients based on the GPT expressions consist of two different effects:

- direct effects: due to the perturbation of cross sections appearing directly in the response function.
- indirect effects: due to the perturbation of neutron flux, caused by the cross sections perturbation.

These effects have been calculated separately with Serpent. Figs. 8-11. show the sensitivity coefficients per unit lethargy of the one-group σ_{fiss} and σ_{capt} to the uncertainty main contributors. As showed in the figures, all these response functions are influenced both directly and indirectly by the considered reactions. In particular it should be noted that:

- the direct terms, plotted in red, are positive, because the one-group cross sections are directly increased by an increase in the cross section data.

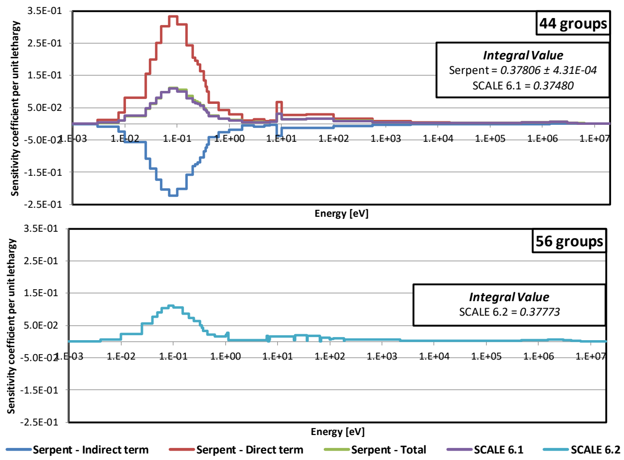

Fig. 8. Sensitivity coefficient of $\sigma_{fiss,\ U235}$ to ^{235}U (n,fiss)

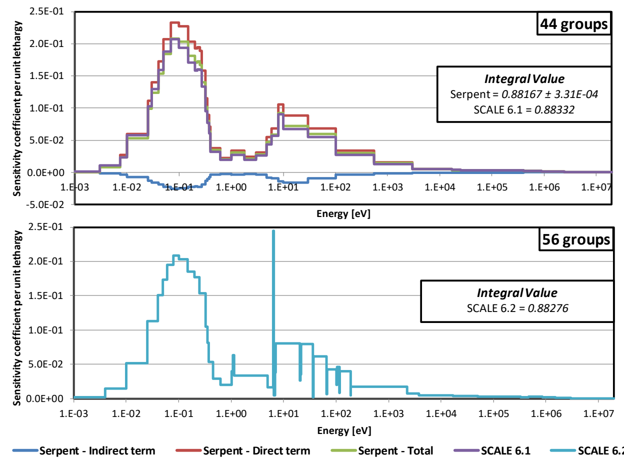

Fig. 9. Sensitivity coefficient of $\sigma_{capt,\ U235}$ to ^{235}U (n,γ)

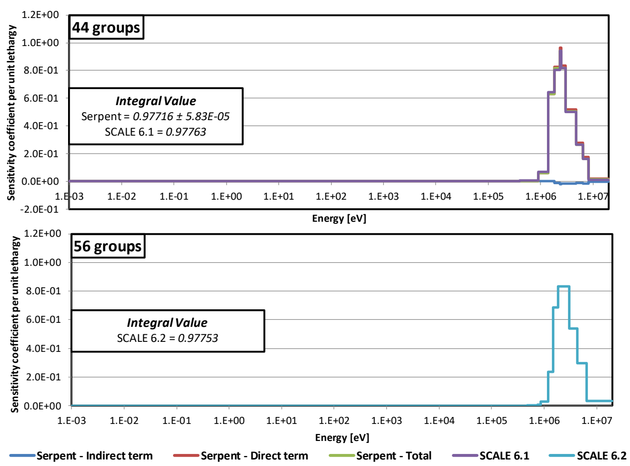

Fig. 10. Sensitivity coefficient of $\sigma_{fiss,\ U238}$ to ^{238}U (n,fiss)

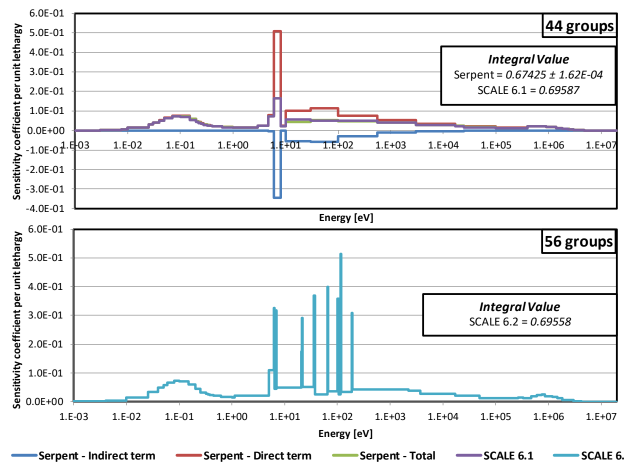

Fig. 11. Sensitivity coefficient of $\sigma_{capt,\ U238}$ to ^{238}U (n,γ)

- the indirect terms, plotted in blue, are negative, because an increase in the cross section data enhances the neutron flux depression causing a decrease of the one-group cross sections.

Serpent-GPT integral sensitivity coefficients show to be in good agreement with SCALE 6.1 and 6.2 ones. The relative errors between the integral values in the three calculations are below 0.9% for the majority of the reactions, except for $\sigma_{capt,\ U238}$ where is approximately 3%. The reason of this difference is similar to that for k_{eff} and should be sought in the implicit sensitivity coefficient calculation in SCALE.

Tables IV-XII show the total uncertainty and main contributors for one-group microscopic cross section of ^{235}U and ^{238}U. In general, Serpent and SCALE 6.1 calculations are in good agreement, while SCALE 6.2 calculation exhibits differences for ^{1}H (n,el), ^{235}U and ^{238}U χ. As already discussed for the k_{eff}, the reason of these differences is due to the new 56 groups covariance matrices of SCALE 6.2.

It should be noted that reactions that contribute both directly and indirectly to the uncertainty are always in the top five contributors, except for the $\sigma_{fiss,\ U235}$, because uncertainty in this reaction is quite small. ^{238}U (n,n') is always one of the top contributors to the uncertainty, because it affects the neutron spectrum and it is quite difficult to be accurately measured.

Table V. Total Uncertainty on $\sigma_{capt, U235}$

Serpent 44 groups		SCALE 6.1 44 groups		SCALE 6.2 56 groups	
$\sigma_{capt, U235}$	Total RSD	$\sigma_{capt, U235}$	Total RSD	$\sigma_{capt, U235}$	Total RSD
8.26E+00 ± 4E-05	1.75 %	8.30E+00	1.77%	8.29E+00	1.76%

Table VI. Main contributors to $\sigma_{capt, U235}$ uncertainty

Covariance Matrix		Serpent 44 groups Relative standard deviation	SCALE 6.1 44 groups Relative standard deviation	SCALE 6.2 56 groups Relative standard deviation
^{235}U (n,γ)	^{235}U (n,γ)	1.284%	1.294%	1.171%
^{238}U (n,n’)	^{238}U (n,n’)	0.962%	0.946%	0.960%
^{235}U χ	^{235}U χ	0.447%	0.444%	0.750%
^{1}H (n,el)	^{1}H (n,el)	0.413%	0.411%	0.215%
^{235}U (n,fiss)	^{235}U (n,γ)	0.340%	0.340%	0.340%

Table VII. Total Uncertainty on $\sigma_{fiss, U235}$

Serpent 44 groups		SCALE 6.1 44 groups		SCALE 6.2 56 groups	
$\sigma_{fiss, U235}$	Total RSD	$\sigma_{fiss, U235}$	Total RSD	$\sigma_{fiss, U235}$	Total RSD
3.52E+01 ± 5E-05	1.15 %	3.53E+01	1.14%	3.52E+01	1.25%

Table VIII. Main contributors to $\sigma_{fiss, U235}$ uncertainty

Covariance Matrix		Serpent 44 groups Relative standard deviation	SCALE 6.1 44 groups Relative standard deviation	SCALE 6.2 56 groups Relative standard deviation
^{238}U (n,n’)	^{238}U (n,n’)	0.930%	0.918%	0.931%
^{235}U χ	^{235}U χ	0.433%	0.430%	0.725%
^{1}H (n,el)	^{1}H (n,el)	0.409%	0.407%	0.241%
^{238}U (n,γ)	^{238}U (n,γ)	0.200%	0.211%	0.216%
^{235}U (n,γ)	^{235}U (n,γ)	0.172%	0.172%	0.166%

Table IX. Total Uncertainty on $\sigma_{capt, U238}$

Serpent 44 groups		SCALE 6.1 44 groups		SCALE 6.2 56 groups	
$\sigma_{capt, U238}$	Total RSD	$\sigma_{capt, U238}$	Total RSD	$\sigma_{capt, U238}$	Total RSD
8.14E-01 ± 6E-05	1.38 %	8.35E-01	1.39%	8.27E-01	1.50%

Table X. Main contributors to $\sigma_{capt, U238}$ uncertainty

Covariance Matrix		Serpent 44 groups Relative standard deviation	SCALE 6.1 44 groups Relative standard deviation	SCALE 6.2 56 groups Relative standard deviation
^{238}U (n,n’)	^{238}U (n,n’)	0.919%	0.902%	0.914%
^{238}U (n,γ)	^{238}U (n,γ)	0.844%	0.877%	0.901%
^{235}U χ	^{235}U χ	0.444%	0.437%	0.735%
^{1}H (n,el)	^{1}H (n,el)	0.362%	0.361%	0.149%
^{235}U (n,γ)	^{235}U (n,γ)	0.064%	0.065%	0.052%

Table XI. Total Uncertainty on $\sigma_{fiss,\ U238}$

Serpent 44 groups		SCALE 6.1 44 groups		SCALE 6.2 56 groups	
$\sigma_{fiss,\ U238}$	Total RSD	$\sigma_{fiss,\ U238}$	Total RSD	$\sigma_{fiss,\ U238}$	Total RSD
1.02E-01 ± 7E-05	4.01%	1.01E-01	3.96%	1.01E-01	4.91%

Table XII. Main contributors to $\sigma_{fiss,\ U238}$ uncertainty

Covariance Matrix		Serpent 44 groups Relative standard deviation	SCALE 6.1 44 groups Relative standard deviation	SCALE 6.2 56 groups Relative standard deviation
^{238}U (n,n’)	^{238}U (n,n’)	3.273 %	3.222%	3.231%
^{235}U χ	^{235}U χ	2.200 %	2.198%	3.623%
^{1}H (n,el)	^{1}H (n,el)	0.518 %	0.513%	0.202%
^{238}U (n,fiss)	^{238}U (n,fiss)	0.509 %	0.510%	0.510%
^{238}U χ	^{238}U χ	0.166 %	0.166%	0.569%

V. CONCLUSIONS

The main objective of this study was to show the capabilities of the Monte Carlo code Serpent in sensitivity and uncertainty analysis, comparing Serpent results with SCALE 6.1 and 6.2. Moreover, the new 56 groups covariance library available in SCALE 6.2 was tested. The TMI pin of the UAM benchmark was chosen as test case.

Results show a very good agreement between Serpent, SCALE 6.1 and 6.2 sensitivity calculations. Concerning the k_{eff}, the relative errors between the integral values in the three calculations were below 0.75% for the majority of the reactions, except for ^{238}U (n, n’) (more neutron histories to improve the results) and ^{238}U (n, γ) (the treatment of implicit effects of SCALE). Concerning the one-group σ, The relative errors between the integral values in the three calculations were below 0.9% for the majority of the reactions, except for $\sigma_{capt,\ U238}$ (again due to the implicit sensitivity coefficient calculation in SCALE).

In general uncertainty calculation with 44 and 56 groups covariance matrices were in good agreement. Some discrepancies were found in the contributions of ^{235}U nubar, ^{235}U and ^{238}U χ and ^{1}H (n,el). This is only due to the updates in the new 56 groups covariance matrices of SCALE 6.2, showing that the contribution of these reactions is changed from the 44 groups covariance libraries.

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