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THE UNIVERSITY OF PISA CALCULATIONS FOR THE PHASE I OF THE OECD/NEA UAM BENCHMARK

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ABSTRACT

In this paper we present the University of Pisa preliminary results for the first exercise of the Phase I of the OECD/NEA Benchmark on the Uncertainty in Analysis and Modeling. The scope of exercise one is to address the uncertainties due to the basic nuclear data as well as the impact of processing the nuclear and covariance data, selection of multi-group structure and self-shielding treatment. DRAGON code and TSUNAMI code were employed, using the available covariance data matrix. The execution of DRAGON calculations required the use of ANGELO and LAMBDA codes for the extension of the covariance matrix from the original SCALE 44 group structure to DRAGON 69 group structure. The uncertainties for the main cross sections were evaluated and are presented here.

Key Words: Covariance, Cross Section Uncertainties, TSUNAMI code, DRAGON code, SCALE codes package

1. INTRODUCTION

In the framework of the Phase I of the OECD/NEA Benchmark for Uncertainty Analysis in Modelling (UAM) [1], the San Piero a Grado Nuclear Research Group (GRNSPG) of the University of Pisa (UNIPI) is performing a series of neutronics calculations aimed to quantify the uncertainties related to the microscopic and macroscopic cross-section libraries and to the core criticality calculation. The selected codes for the first two exercises of the Phase I of the benchmark were the TSUNAMI [2] & NEWT [3] codes of the SCALE5.1 codes package [4] and the DRAGON lattice physics code [5].

2. THE EXERCISE I-1: THE CELL PHYSICS CALCULATIONS MODELING

The aim of the Exercise I-1 is to address the uncertainties due to the basic nuclear data as well as the impact of processing the nuclear and covariance data, selection of multi-group structure and self-shielding treatment. The estimation of these uncertainties should then be propagated, during the Exercise I-2, into the macroscopic cross section libraries generation process.

In order to analyze several reactor models, different elementary fuel cells were considered: Three Mile Island-1 (TMI-1) PWR and Peach Bottom-2 (PB-2) BWR fuel cells (see Fig. 1), and the Kozloduy-6 VVER fuel cell.

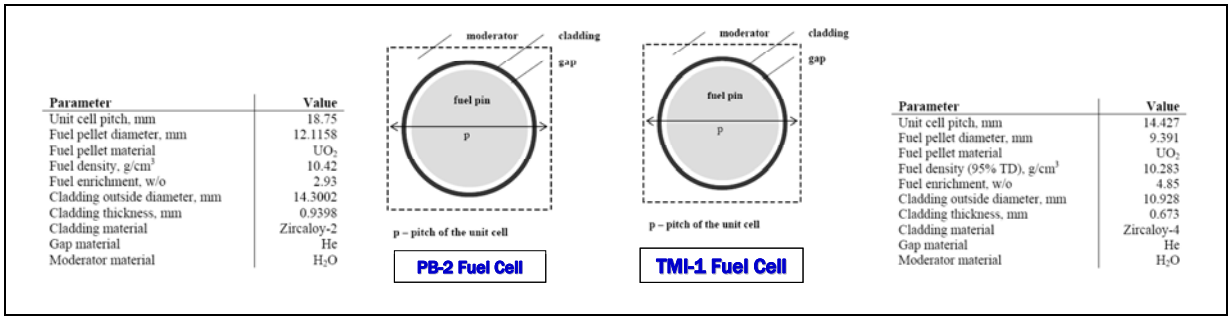

Figure 1 – Different LWR Fuel Cell models for the UAM Exercise I-1

The benchmarks participants were asked to perform multi-group transport cell calculations of these elementary systems, using the mesh energy resolution of their transport code. Thus, the obtained, multi-group fluxes had to be used to weight the self-shielded microscopic cross sections used for calculations according to the definition (1) :

$$\alpha_i = \frac{\overline{\sigma}_i \overline{\phi}_i}{\overline{\sigma}\overline{\phi}_T} \qquad (1),$$

where *i* indicates an energy group. Each of these parameters were calculated for the most relevant isotopes and then used for calculating the effective uncertainty (relative error) for the cross sections using the formula (2):

$$\Delta^2 = \sum_{i \in n, j \in n} \alpha_i \, \mathrm{cov}(i, j) \alpha_j \qquad (2)$$

It should be noted that four different covariance libraries were supplied by the benchmarks organizers, in particular:

- 44GROUPV5COV, basic ENDF/B-V Covariance Library
- 44GROUPV5REC, recommended ENDF/B-V Covariance Library
- 44GROUPV6COV, basic ENDF/B-VI Covariance Library
- 44GROUPV6REC, recommended ENDF/B-VI Covariance Library

Two calculations schemes were set up, one based on the TSUNAMI code of the SCALE5.1 codes package, the other one on the DRAGON lattice physics code. The TSUNAMI calculations hereafter reported were executed using the second covariance library, the 44GROUPV5REC. Conversely, DRAGON calculations were performed using the fourth covariance library, 44GROUPV6REC. Fig. 2 and Fig. 3 show the calculation flows for each scheme.

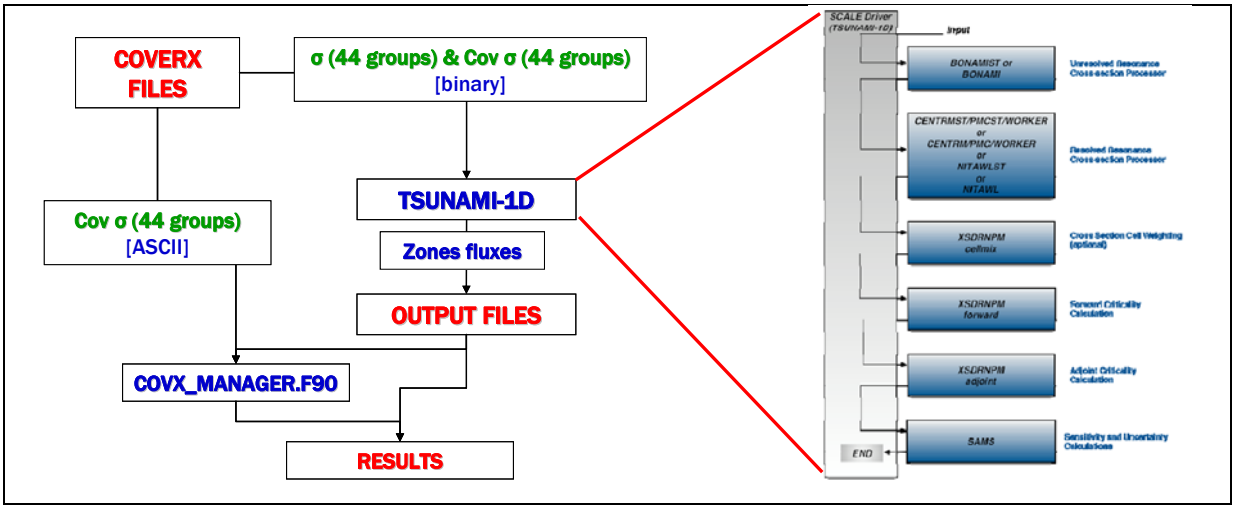

Figure 2 – The TSUNAMI code based calculation scheme for the UAM Exercise I-1

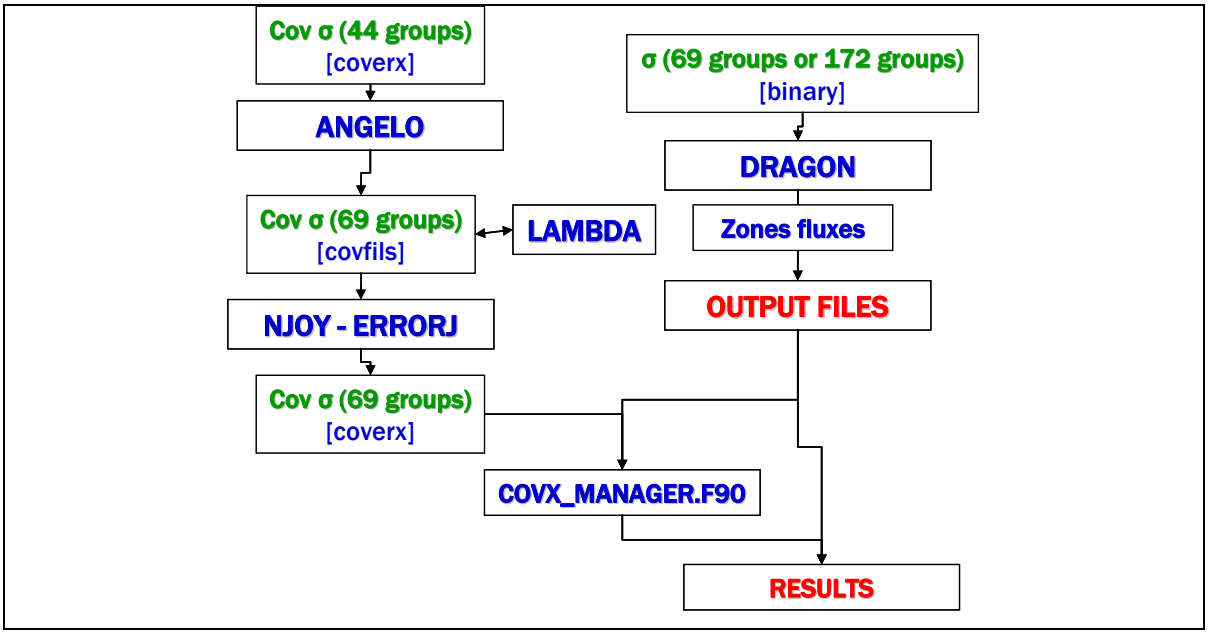

Figure 3 – The DRAGON code 69 groups based calculation scheme for the UAM Exercise I-1

Using the TSUNAMI code, it was not necessary to modify the covariance library energy group structure (i.e., TSUNAMI is using a 44 energy groups ENDF/B-VI based library). The DRAGON code, however, required a transformation from the library's native 44 group structure to the 69 and 172 group structures used by DRAGON. In fact, GRNSPG is using the DRAGON code with the IAEA WIMS-D updated libraries, which have a greater energy resolution. The process of transforming the covariance matrix from 44 to 69 and 172 was completed using the

ANGELO code [6]. Verification of the transformed covariance matrices was performed by the LAMBDA code [6], to ensure that the covariance has not been corrupted as a result of the transformation procedure. Both the ANGELO and LAMBDA codes were supplied by the benchmarks organizers.

The sequence of calculation modules that was used for the TSUNAMI code was: BONAMIST (Unresolved resonance cross section processor) – NITAWLST (resolved resonance cross section processor) – XSDRNPM (1D forward/adjoint criticality calculations). For the DRAGON code, the calculation modules employed were: EXCELT (geometry tracking) – SHI (self-shielding using Stammler approximation) – ASM/FLU (forward flux calculation using collision probability matrix) – SAD (adjoint calculation).

3. THE EXERCISE I-1: THE CELL PHYSICS CALCULATIONS RESULTS

Calculations of the multi-group neutron flux and the relative uncertainties are presented here for the PB-2 BWR fuel cell, TMI-1 fuel cell and Kozloduy-6 fuel cell. All calculations were executed using as boundary and initial conditions the benchmark specifications (see Fig.1). The results are given in Table I.

Table I – Criticality calculations by the TSUNAMI & DRAGON codes for the fuel cell simulations

	TSUNAMI (44 groups)		DRAGON (69 groups)	
Fuel Cell	**Forward**	**Adjoint**	**Forward**	**Adjoint**
TMI-1	1.423671	1.423662	1.426044	1.42590
PB-2	1.338558	1.338547	1.339906	1.33291
Kozloduy-6	1.331494	1.331570	1.344591	1.34459

TSUNAMI code allowed for the automatic calculation of sensitivity parameters for the k_{inf} and to visualize them as function of the energy by the use of JAVAPENO plotting tool. Example of results from these sensitivities calculations for both TMI-1 and PB-2 fuel cells are given in Figure 4 and Figure 5.

Mixture	Nuclide	Atom Density	Sensitivity
1	235U	6.90E-04	1.58E-01
4	1H	5.04E-02	1.22E-01
3	114Sn	3.14E-06	-5.26E-06
3	122Sn	2.23E-05	-6.91E-06
3	112Sn	4.68E-06	-2.70E-05
3	124Sn	2.79E-05	-3.51E-05
3	115Sn	1.74E-06	-5.71E-05
3	120Sn	1.57E-04	-5.93E-05
3	119Sn	4.14E-05	-8.53E-05
3	Ni	3.70E-05	-1.19E-04
3	116Sn	7.01E-05	-1.40E-04
3	118Sn	1.17E-04	-1.40E-04
3	Cr	7.60E-05	-1.62E-04
3	Fe	9.55E-05	-1.69E-04
3	117Sn	3.71E-05	-1.72E-04
1	234U	1.28E-06	-5.04E-04
3	Hf	2.21E-06	-7.56E-04
2	4He	1.50E-01	-7.99E-04
4	16O	2.52E-02	-2.46E-03
3	Zr	4.26E-02	-1.26E-02
1	16O	4.65E-02	-1.31E-02
1	238U	2.26E-02	-2.08E-01

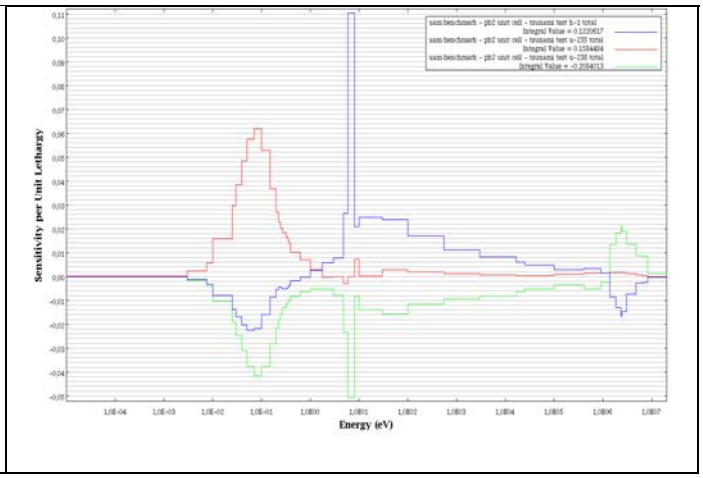

Figure 4 – Sensitivity calculations for PB-2 Fuel Cell

Mixture	Nuclide	Atom Density	Sensitivity
4	1H	5.12E-02	1.37E-01
1	235U	1.13E-03	1.02E-01
3	114Sn	3.14E-06	-4.08E-06
3	122Sn	2.23E-05	-5.42E-06
3	112Sn	4.68E-06	-2.28E-05
3	124Sn	2.79E-05	-3.01E-05
3	115Sn	1.74E-06	-3.46E-05
3	120Sn	1.57E-04	-4.90E-05
3	119Sn	4.14E-05	-5.82E-05
3	Cr	7.60E-05	-1.00E-04
3	116Sn	7.01E-05	-1.24E-04
3	118Sn	1.17E-04	-1.24E-04
3	117Sn	3.71E-05	-1.35E-04
3	Fe	1.49E-04	-1.64E-04
1	234U	1.26E-06	-4.12E-04
2	4He	1.50E-01	-5.79E-04
3	Hf	2.21E-06	-6.04E-04
4	16O	2.56E-02	-2.86E-03
3	Zr	4.25E-02	-1.00E-02
1	16O	4.59E-02	-1.17E-02
1	238U	2.18E-02	-1.71E-01

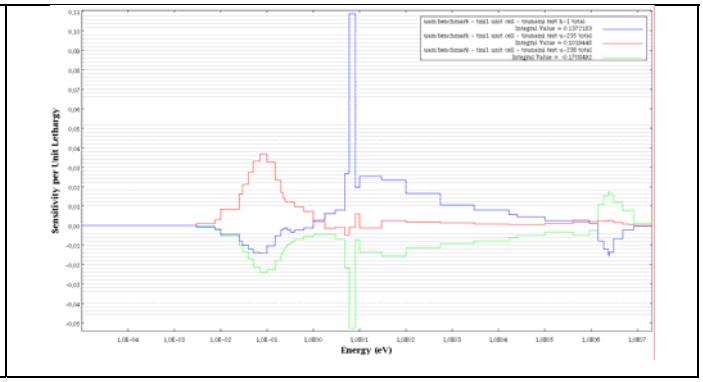

Figure 5 – Sensitivity calculations for TMI-1 Fuel Cell

It is worthwhile to note that the most important nuclides affecting the k_{inf} are (as expected) U238, hydrogen and U235. A further investigation about which nuclear reaction contributed to the k_{inf} uncertainty was also conducted by the TSUNAMI code, e.g. resulting in the Table II for the PB-2 fuel cell. A similar table was also obtained for the TMI-1 and Kozloduy-6 fuel cells. The relative and absolute standard deviations of k_{inf} for all three cells are reported in Table III.

Table II – Relative and Absolute Standard deviation of k_{inf}

Covariance Matrix		Contributions to Uncertainty in keff (% dk/k)
Nuclide-Reaction	Nuclide-Reaction	Due to this Matrix
235U nubar	235U nubar	6.19E-01
238U n,gamma	238U n,gamma	5.71E-01
235U n,gamma	235U n,gamma	3.61E-01
1H elastic	1H elastic	1.57E-01
235U fission	235U fission	1.52E-01
Zr n,gamma	Zr n,gamma	7.71E-02
238U n,n'	238U n,n'	7.38E-02
235U chi	235U chi	7.20E-02
238U fission	238U fission	6.65E-02
238U nubar	238U nubar	5.08E-02
16O n,alpha	16O n,alpha	4.29E-02
1H n,gamma	1H n,gamma	3.39E-02
238U n,n'	238U fission	1.72E-02
16O elastic	16O elastic	1.37E-02
Zr n,n'	Zr n,n'	1.36E-02
238U chi	238U chi	1.13E-02
238U n,n'	238U n,gamma	-9.36E-03
238U n,2n	238U n,2n	8.94E-03
238U elastic	238U n,gamma	7.09E-03
238U n,n'	238U elastic	-5.60E-03
238U n,n'	238U n,2n	4.78E-03
16O elastic	16O n,alpha	-4.16E-03
16O n,n'	16O n,n'	3.78E-03
234U n,gamma	234U n,gamma	3.45E-03
118Sn n,gamma	118Sn n,gamma	2.55E-03

Table III – Relative and Absolute Standard deviation of k_{inf}

	TSUNAMI code	
Fuel Cell	**Relative**	**Absolute**
TMI-1	1.0160%	1.4464%
PB-2	0.9567%	1.2806%
Kozloduy -6	0.9855%	1.3129%

The final part of the Exercise I-1 was devoted to the calculations of the relative errors resulting from the cross section uncertainties and from the transport calculations. Calculations of these relative errors were performed using the formula (2), and reported in the Table IV for the TMI-1 fuel cell.

Table IV – Relative errors for some of the most important nuclides of the TMI-1 fuel cell

Reaction	Δ^2
H-1-elastic to H-1-elastic	3.1600E-02
H-1-n,gamma to H-1- n,gamma	2.3419E-06
H-1-total to H-1-total	3.1729E-02
H-1-total to H-1-elastic	3.1664E-02
H-1-total to H-1-n,gamma	6.1753E-07
U-235-nubar to U-235-nubar	2.0167E-04
U-235-chi to U-235-chi	7.0066E-04
U-238-elastic to U-238-elastic	2.0956E-02
U-238-n,n' to U-238- n,n'	4.8333E-02
U-238-n,2n to U-238- n,2n	3.6522E-03

It can be seen how the most relevant errors are introduced by some of the H-1, U-235 and U-238 nuclear reaction cross sections.

One-group microscopic cross-sections for several isotopes of interest, including their associated relative uncertainties were calculated with DRAGON code too (see Fig. 6), using the aforementioned extrapolated 69-group covariance matrices. These one-group cross sections and uncertainties are shown in Table V; all cross sections are reported in units of barns. For some isotope-reaction pairs, namely U-234 fission, insufficient covariance data was available at the time of the calculations to determine uncertainties.

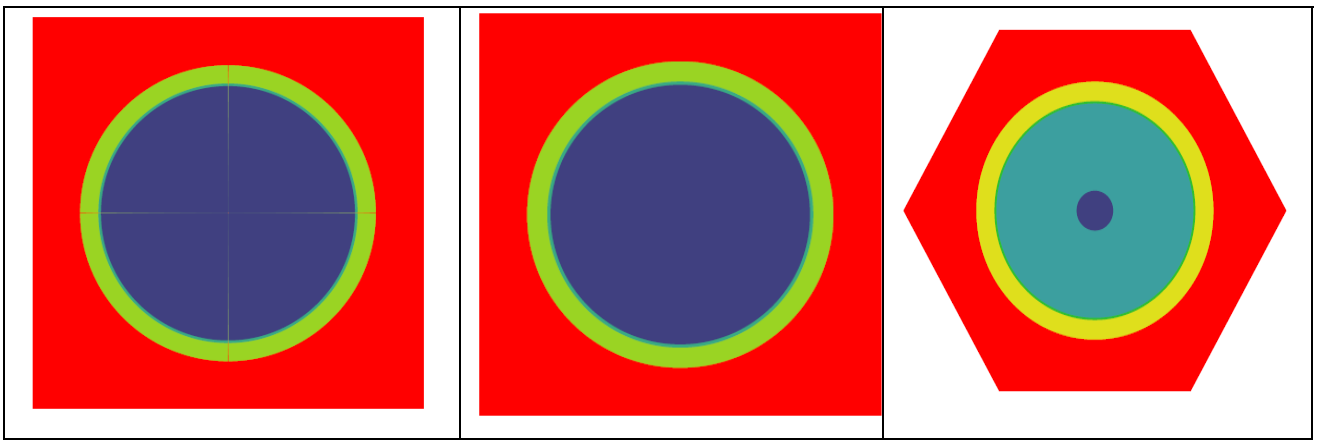

Figure 6 – DRAGON model for TMI-1, PB-2 and Kozloduy-6 fuel cells

Table V – One-group cross-sections and associated uncertainties for selected reactions

TMI-1	$\sigma_{CAPTURE}$	$\sigma_{FISSION}$	Δ	Δ^2
U-234	1.8786E+01	------	7.8461E-02	6.1561E-03
U-234	------	5.0253E-01	no data	no data
U-235	8.0309E+00	------	1.7443E-02	3.0425E-04
U-235	------	3.5150E+01	3.9113E-03	1.5298E-05
U-238	8.3116E-01	------	2.0281E-02	4.1133E-04
U-238	------	1.0379E-01	1.1200E-02	1.2543E-04
PB-2	$\sigma_{CAPTURE}$	$\sigma_{FISSION}$	Δ	Δ^2
U-234	2.1051E+01	------	6.8874E-02	4.7437E-03
U-234	------	4.7211E-01	no data	no data
U-235	1.0501E+01	------	1.4007E-02	1.9619E-04
U-235	------	4.9461E+01	3.0474E-03	9.2868E-06
U-238	8.4219E-01	------	1.9713E-02	3.8859E-04
U-238	------	9.6775E-02	1.1322E-02	1.2819E-04
Kozloduy-6	$\sigma_{CAPTURE}$	$\sigma_{FISSION}$	Δ	Δ^2
U-234	2.1230E+01	------	7.0463E-02	4.9650E-03
U-234	------	4.7251E-01	no data	no data
U-235	1.0362E+01	------	1.452E-02	2.1087E-04
U-235	------	4.8203E+01	3.1529E-03	9.9409E-05
U-238	9.1631E-01	------	2.0430E-02	4.1738E-04
U-238	------	9.7117E-02	1.1547E-02	1.3334E-04

4. THE APPROACH FOR EXERCISE I-2

Exercise I-2 is focused on the propagation of input uncertainties through lattice physics calculations to output uncertainties in evaluated lattice-averaged parameters. The input uncertainties will be the multi-group cross-section uncertainties calculated above, the uncertainties associated with methods and modeling approximation and finally the fuel assembly manufacturing uncertainties.

The GRNSPG/UNIPI approach will be to propagate the multi-group input uncertainties to the 2 group homogenous cross sections using calculated sensitivity coefficients for the 2 group cross sections libraries and the multi group covariance matrices. In this way a 2 group covariance matrix for the homogeneous macroscopic cross sections will be obtained, allowing an estimation of one/two group effective uncertainties. Mini-core results will also allow estimation the effect of spatial and energetic homogenization.

Also for this exercise, two codes, the DRAGON code and the NEWT 2D transport code of the SCALE codes package, will be used, in order to have independent results.

5. CONCLUSIONS

Preliminary calculations of Exercise I-1 of the OECD/NEA UAM benchmark have been presented. The GRNSPG/UNIPI is carrying out these exercises using two independent codes (DRAGON and TSUNAMI/SCALE). The identification of the main nuclides and of the main nuclear reaction uncertainties contributing to the global fuel cell uncertainties has been carried out. The outline of the procedure that will be used for the execution of the successive step (propagation of the multi-group cross section uncertainties to the few group cross sections) has also been described. Current works are focusing on the check-up of the whole procedures.

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