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Nuclear Data Uncertainty Propagation in Reactor Studies Using the SANDY Monte Carlo Sampling Code

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Abstract - *A Monte Carlo sampling code called SANDY for the nuclear data uncertainty propagation is described and tested against several reactor case studies. SANDY can efficiently read and process nuclear data files in the ENDF-6 format, commonly adopted for the storage and retrieval of evaluated nuclear data for applications of nuclear technology.*
In this work, SANDY is used to sample and propagate the covariance data available in ENDF-6 files. The uncertainties of multiple reactor responses are quantified, such as integrated cross sections, k_∞, k_{eff}, β_{eff}, reactivity worths and damage metrics. The reactor models taken into considerations were the VENUS-F fuel assembly with solid bismuth blocks and plates, a scale-down version of the ASTRID sodium fast reactor operated as a minor actinide burner and the MYRRHA multi-purpose facility in subcritical mode.
Results show the flexibility of SANDY in propagating multiple uncertainties to different nuclear responses. Also, conclusions were drawn on the reliability of the current evaluated covariance data available.

I. INTRODUCTION

The major efforts made by the nuclear data evaluators community in producing covariance matrices for many nuclear parameters promoted the use of the "BEPU" approach (best estimate + uncertainty) in nuclear practices ranging from design, to licensing and operation. In this context, several institutes have recently developed computer codes for the nuclear data uncertainty propagation via Monte Carlo sampling. Amongst them, one could mention NUDUNA [1], SAMPLER [2] and TMC [3].

A new nuclear data sampling code SANDY (SAmpling of Nuclear Data and uncertaintY) has been developed at SCK•CEN [4]. SANDY relies on stochastic sampling to propagate nuclear data covariances, which are retrieved from input files in ENDF-6 format [5]. SANDY is model-independent and can operate with any solver in a "black-box" approach, provided that the solver is compatible with the ENDF-6 format input files, either directly or via data processing. SANDY aims at handling all the covariance sections of the ENDF-6 format. In addition, variance-based sensitivity analysis capabilities were added to the code.

In the first part of this paper we provide a description of SANDY, listing its many features for uncertainty propagation and sensitivity analysis. The second part reports the application of SANDY to quantify the uncertainty of integral responses for various nuclear systems. SANDY was applied to nuclear models that characterize the behavior of fast reactors. First, energy-dependent global sensitivity coefficients were assessed for the ^{23}Na elastic scattering integrated cross section, which plays an important role for the neutronics of sodium reactors, as highlighted in the next sections. Second, the uncertainty of the infinite neutron multiplication factor k_∞ was evaluated for an individual fuel assembly of the VENUS-F facility [6]. Then, uncertainties were quantified for the effective neutron multiplication factor k_{eff} and reactivity feedback coefficients in the full core model of a sodium fast reactor (SFR). The last study involved the uncertainty quantification of radiation damage metrics for ^{184}W in the irradiation conditions of the MYRRHA subcritical reactor [7].

II. INSIGHT OF THE SANDY CODE

1. Nuclear data sampling

SANDY is a nuclear data sampling tool applicable to sensitivity analysis (SA) and uncertainty quantification (UQ) problems. The code exploits the basic theory of Monte Carlo sampling to propagate nuclear data covariances through the nuclear models under study. The best-estimates and covariance information that act as input of SANDY must be provided in the ENDF-6 format [5]. Below are the processing steps implemented in SANDY to produce nuclear data random files:

1. retrieve best-estimates $\boldsymbol{\mu}$ and covariance matrix $\boldsymbol{\Sigma}$ from ENDF-6 files;
2. from $\boldsymbol{\Sigma}$ extract correlation matrix $\boldsymbol{C}$ and standard deviations $\boldsymbol{\sigma}$;
3. apply Cholesky decomposition to the correlation matrix, $\boldsymbol{C} = \boldsymbol{L}\boldsymbol{L}^\top$;
4. draw $\mathcal{N}(0, 1)$ random uncorrelated samples $\boldsymbol{x}_{\mathcal{N}(\mathbf{0},\mathbf{1})}$;
5. apply correlations in $\boldsymbol{C}$ to the uncorrelated samples: $\boldsymbol{x}_{\mathcal{N}(\mathbf{0},\boldsymbol{C})} = \boldsymbol{L}\boldsymbol{x}_{\mathcal{N}(\mathbf{0},\mathbf{1})}$;
6. adjust samples by best-estimates and standard deviations: $\boldsymbol{x}_{\mathcal{N}(\boldsymbol{\mu},\boldsymbol{\Sigma})} = \boldsymbol{\mu} + \boldsymbol{\sigma} \circ (\boldsymbol{L}\boldsymbol{x}_{\mathcal{N}(\mathbf{0},\mathbf{1})})$;
7. write nuclear data samples into ENDF-6 format perturbed files.

The working scheme of SANDY is also reported in Figure 1.

The random files can be used by any nuclear code that is compatible with the ENDF-6 format, either directly or via data conversion. Then, the Monte Carlo uncertainty propagation

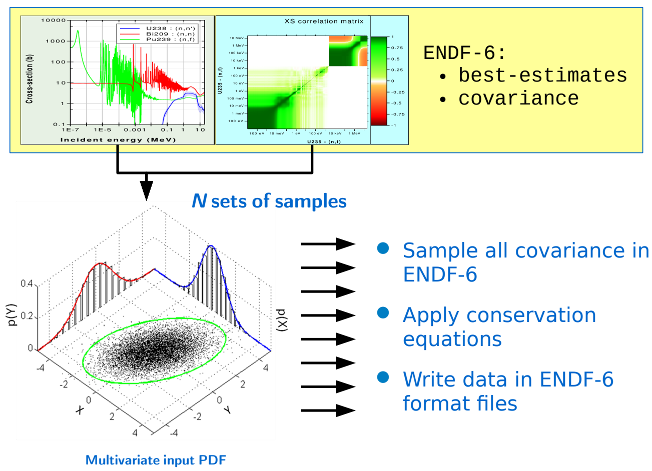

Fig. 1. SANDY's working scheme.

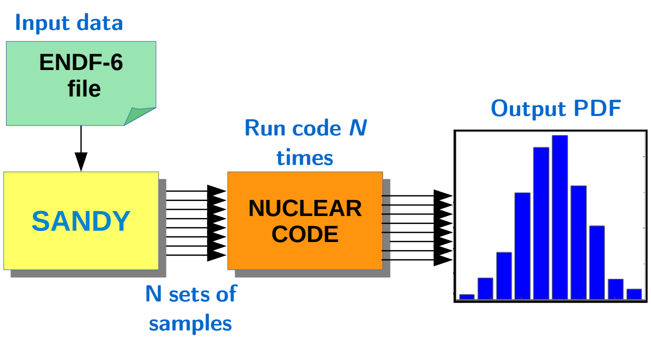

Fig. 2. Monte Carlo uncertainty propagation scheme using SANDY.

can be carried out on the nuclear code's several responses, as illustrated in Figure 2.
SANDY can sample the following ENDF-6 nuclear data:

- fission neutron multiplicities (MF=31);
- resonance parameters (MF=32);
- cross sections (MF=33);
- angular distributions of secondary particles (MF=34);
- energy distributions of secondary particles (MF=35);
- radioactive decay data (MF=8);
- fission yields (MF=8).

In brackets we reported the ENDF-6 section number where the covariance / uncertainty data are stored.

Since the covered test cases include only neutronics studies, few extra details are reported for the sampling of the nuclear data that appear in these calculations.

Fission neutron multiplicities

Samples for the total fission neutron multiplicity $\overline{\nu}_{tot}$ are not drawn from the corresponding covariance matrix, but are rather calculated from the samples of the prompt and delayed multiplicities — i.e. $\overline{\nu}_p$ and $\overline{\nu}_d$, respectively — applying the conservation equation:

$$\overline{\nu}_{tot} = \overline{\nu}_p + \overline{\nu}_d \, . \tag{1}$$

Resonance parameters

In the resolved resonance region (RRR), samples are drawn for resonance parameters represented by single- or multi-level Breit-Wigner (SLBW and MLBW), Reich-Moore (RM) and R-matrix limited format. SANDY does not handle covariance matrices for resonances in the unresolved resonance region (URR) as it is unclear how to establish a rigorous way to perturb the energy dependent parameters [5]. Only for resonance parameters, SANDY gives the user the possibility to sample from a LogNormal multivariate distribution.

Cross sections

The ENDF-6 format allows two types of sections in MF=33: NI-type and NC-type sections. NI-type sections provide explicit cross section covariances, which are represented as stepwise functions of energy and are mostly expressed in relative values. NC-type sections describe the rules to derive specific cross sections as a linear combination of other cross sections with a covariance matrix. SANDY draws samples from a global covariance matrix that incorporates all the NI-type covariances for the many cross sections of a single isotope. Each of these samples is centered in zero and represents a relative perturbations of a specific cross section, to be applied to any tabulated value within the energy interval corresponding to the step of the covariance function. Then, SANDY applies the combination rules retrieved from the NC-type sections. Eventually, SANDY reintroduces consistency in the samples by applying the summation rules of redundant reactions.

Angular distributions

According to the ENDF-6 format, covariances for the angular distributions are provided only between Legendre coefficients, even for the cases where the angular distribution is expressed as a tabulated probability distribution.

Energy distributions

Although five representations are available for the secondary neutron energy distributions — i.e. tabulated form, Maxwellian fission spectrum, evaporation spectrum, Watt spectrum, Madland and Nix spectrum — SANDY only samples data in tabulated energy distributions, since the current releases of the major nuclear data libraries do not provide covariance matrices for distributions in other forms. Then, for each samples distribution, SANDY applies a normalization to unit.

2. Global sensitivity analysis

SANDY relies on the theory of ANOVA (ANalysis Of VAriance) [8] for uncorrelated and correlated parameters to determine estimates of global sensitivity coefficients.

According to ANOVA, the response variance V_y of a functional $y = f(\boldsymbol{x})$ can be expanded as

$$V_y = \sum_{i=1}^{n} V_i + \sum_{i=1}^{n} \sum_{j>i}^{n} V_{ij} + \cdots + V_{1,\ldots,n}\,, \tag{2}$$

where each term V_i is called variance of the conditional mean and represent the fraction of V_y "explained" by x_i. All the higher order summands include the cooperative contributions of x_i with all the other inputs. For uncorrelated inputs SANDY calculates a *model-free* global sensitivity index

$$S_{T_i} = \frac{V_i + \sum_{j\neq i}^{n} V_{ij} + \cdots + V_{1,\ldots,i,\ldots,n}}{V_y}\,, \tag{3}$$

which describes the total effect of x_i to the variance of y. In contrast to perturbation theory, S_{T_i} can be directly calculated regardless of the magnitude of its nonlinear terms, because of the model-free nature. For correlated parameters, SANDY applies the decorrelation process described in [9] to assess the global sensitivity indices S^c for the correlated effect of x_i and S^u for its uncorrelated effect.

SANDY can calculate global sensitivity indices for single parameters, such as a resonance width, or groups of parameters, such as all the cross sections within an energy interval. In the next chapters the correlated global sensitivity index S^c will be expressed as a function of energy.

III. APPLICATION TO TEST CASES

1. ^{23}Na integrated elastic scattering cross section

To show the capabilities of the code, SANDY was initially tested on a simple mockup problem, such as the uncertainty propagation to an integrated cross section. The chosen response $\langle\sigma_{(n,n)}\rangle$ was the convolution between the ^{23}Na scattering cross section $\sigma_{(n,n)}(E)$ and a weighting function $\phi(E)$ with a fusion peak, intermediate shape typical of a fast reactor and a low thermal part (Figure 3):

$$\langle\sigma_{(n,n)}\rangle = \frac{\int_E \sigma_{(n,n)}(E)\phi(E)dE}{\int_E \phi(E)dE}\,. \tag{4}$$

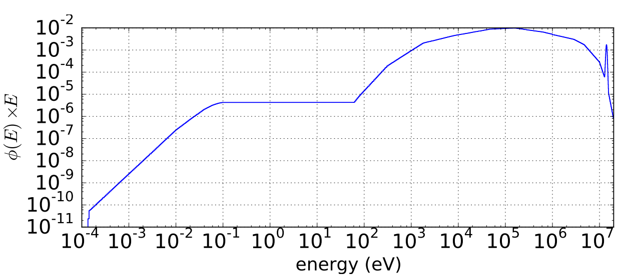

Fig. 3. Weighting function used for the calculation of integrated cross sections.

Because of its magnitude the ^{23}Na elastic scattering cross section is largely responsible for the neutron spectrum thermalization in sodium fast reactors and plays an important role in the characterization of the neutron multiplication factor. For this exercise, only the tabulated ^{23}Na $\sigma_{(n,n)}(E)$ cross section was sampled with SANDY using the tabulated data and covariances in ENDF/B-VII.1 [10] (Figure 4). Although other isotopes/reactions may also contribute to the integrated cross section uncertainty by influencing the neutron flux of the system, they were not taken into account to keep the exercise simple.

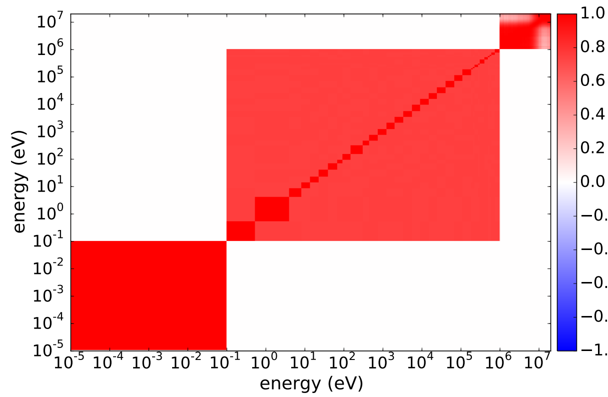

Fig. 4. Correlation matrix of the ^{23}Na energy-dependent differential elastic scattering cross section in ENDF/B-VII.1.

SANDY samples were used in combination with the GROUPR module of NJOY [11] to quantify the mean and standard deviation of the integrated cross section. The uncertainty was also quantified with the module ERRORR of NJOY [11] and results were compared in Table I.

	ERRORR	SANDY
best estimate	7.941	7.940
uncertainty	0.196	0.194

TABLE I. Comparison of the integrated ^{23}Na scattering cross section best estimate and uncertainty calculated with ERRORR and SANDY. 87000 samples were generated with SANDY.

Table I shows that for a large number of samples SANDY and ERRORR produce equivalent results.

Exploiting SANDY's variance decomposition capabilities, global sensitivity indices were assessed for the correlated effect of the differential cross section as a function of energy and are reported in Figure 5. The global sensitivity index profile highlights the energy block structure of the covariance matrix.

2. VENUS-F fuel assembly model

SANDY was tested to quantify the k_∞ uncertainty of a VENUS-F fuel assembly. VENUS-F is a zero power reactor facility at the SCK•CEN site, which uses solid lead to simulate the neutronic behavior of heavy metal liquid coolants of fast reactors [6]. A VENUS-F fuel assembly includes a 5×5 lattice filled with 13 metallic uranium rods, four Al_2O_3 rods and eight cladded lead blocks, and it is surrounded by lead plates (Figure 6). The fuel is enriched in ^{235}U for about 30 wt.%. Consistently with the most recent modifications applied to the VENUS-F core, in this assembly model we replaced the lead blocks and plates with solid bismuth.

A k_∞ of 1.74540 with 8 pcm of statistical error was cal-

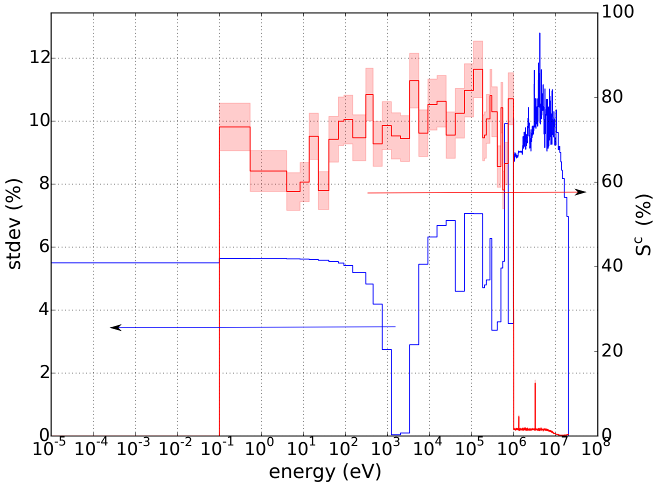

Fig. 5. Correlated effect global sensitivity indices S^c for the integrated ^{23}Na elastic scattering cross section.

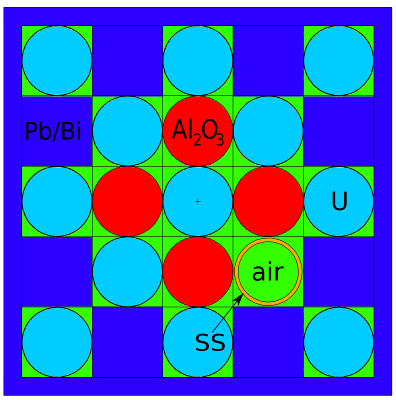

Fig. 6. VENUS-F core model (VFV8-CC5) [12, 13].

culated with MCNP [14] for the described model. Then, the ENDF/B-VII.1 nuclear data covariances for cross sections, prompt fission neutrons multiplicities ($\overline{\nu}_p$) and fission spectra (χ) were propagated with SANDY. A total uncertainty of 5650 pcm was quantified. Uncertainties of this order of magnitude can question the reliability of the whole calculation.

A global sensitivity study was carried out using SANDY. The contribution of the several nuclear data involved to the k_∞ uncertainty was quantified and it is reported in Table II.

	(n,n)	(n,n^*)	(n,f)	(n,γ)	$\overline{\nu}_p$	χ
^{209}Bi	55	133	-	143	-	-
^{235}U	35	273	264	5476	179	393
^{238}U	49	1065	54	308	189	38

TABLE II. Uncertainty contributions in pcm to the VENUS-F fuel assembly k_∞, generated by the covariance data of the several nuclear data involved in the calculation.

It was recognized that almost 5500 pcm of uncertainty sprout from the radiative capture cross section of ^{235}U around 10 keV, where the ENDF/B-VII.1 evaluated cross section uncertainty is larger than 35%, as shown in Figure 7. The cross section evaluated uncertainty in this energy range should be addressed, as it strongly affects uncertainty studies for fast reactors loaded with ^{235}U in great amount.

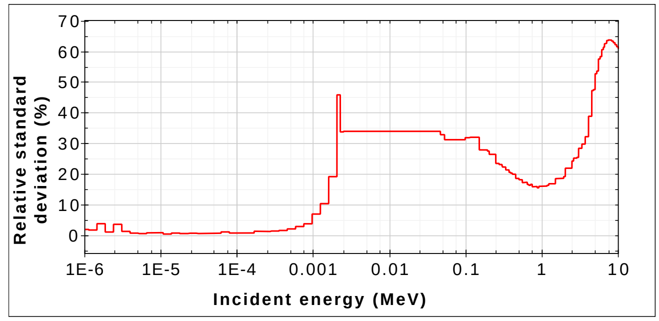

Fig. 7. Relative standard deviation of the ^{235}U radiative capture cross sections of ENDF/B-VII.1.

3. SFR core model

In this section, SANDY was employed to calculate and characterize the uncertainty on the k_{eff}, the effective delayed neutron fraction β_{eff} and the void worth and Doppler effects of an SFR loaded with a large amount of minor actinides (MAs). These parameters quantify some crucial safety measures that a reactor must comply with. Since the absolute values of these major safety parameters are generally lower in MA fueled SFRs than in traditional light water reactors, it is important to assess reliable and accurate uncertainties.

The random sampling was carried out for the ENDF/B-VII.1 neutron cross sections, scattering angular distributions, fission neutrons multiplicities and spectra. Uncertainties were propagated through the criticality calculation of the ASTRID SFR concept, modeled with MCNP following the specifications in [15]. A radial view of the core SFR core is shown in Figure 8.

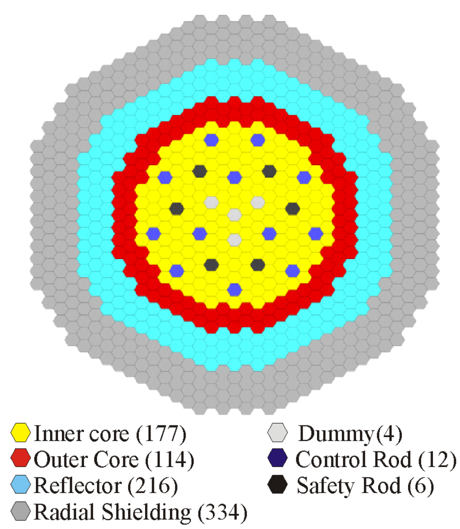

Fig. 8. Radial layout of the SFR MA burner [15].

The choice of fuel served the purpose of modeling a MA burner core and is reported in Table III.

Element	Inner fuel	Outer fuel
U	65.09	62.14
Np	0.46	0.50
Pu	23.28	23.35
Am	10.69	11.64
Cm	0.48	0.53

TABLE III. Atomic fraction (%) of a single element over the total amount of actinides in the fuel zone.

While the choice of depleted uranium and plutonium weight fractions reflects the composition of a typical Mixed OXide (MOX) fuel, the vector of TRans-Uranic elements (TRUs) reproduces the reprocessing product of a Pressurized Water Reactor (PWR) spent fuel after 30 years from irradiation. All best-estimate and uncertainty results are reported in Table IV.

Parameter	Best estimate (pcm)	Uncertainty (pcm)
k_{eff}	1.02086	1827
β_{eff}	266	9
$\Delta\rho_v$ (inner)	414	46
$\Delta\rho_v$ (outer)	1118	71
$\Delta\rho_v$ (extended)	-327	73
$\Delta\rho_d$	-45	6

TABLE IV. Best estimate and uncertainty values of the SFR neutronics and reactivity feedback parameters calculated with MCNP and SANDY.

The uncertainty of the k_{eff} was quantified to 1827 pcm. Then, the contribution generated by several nuclear data parameters were assessed with SANDY and are reported in Table V. It results that the contribution of U-238 data is dominant, i.e. total of 1753 pcm, despite the high content in MAs. If joint efforts aimed at improving the nuclear data for MA burners were to be undertaken, they should primarily focus on the U-238 data at fast energies and in particular on its inelastic cross section. Regarding the minor actinides data contribution, it was found that these isotopes are responsible for 17% of the fissions, and together with Pu they make up to 30% of the total calculated k$_{eff}$ uncertainty. This contribution is significant and should be taken into careful account when designing a MA burner system.

	(n,n)	(n,n^*)	(n,f)	(n,γ)	$\overline{\mu}$	$\overline{\nu}_p$	χ
^{23}Na	52	109	-	-	22	-	-
^{56}Fe	209	212	-	-	26	-	-
^{238}U	57	1185	119	72	-	1227	20
^{239}Pu	244	-	238	206	-	50	181
^{240}Pu	215	111	193	196	-	-	50
^{241}Am	56	-	118	194	-	143	-
^{243}Am	18	-	86	99	-	29	-

TABLE V. Uncertainty contributions in pcm to the SFR MA burner k_{eff}.

In comparison to a traditional MOX fuel, the presence of a large amount of minor actinides translates into a smaller β_{eff}, resulting in the need for stricter safety margins. An overall β_{eff} uncertainty of 9 pcm (3.38%) was found, with significant contribution from the fission prompt neutron multiplicity data of U-238 and Pu-239 (Table VI).

	xs	$\overline{\nu}_p$
^{238}U	1.08	1.93
^{239}Pu	0.58	2.12
^{240}Pu	1.36	-
^{241}Am	0.06	0.11
^{243}Am	0.51	0.41

TABLE VI. Uncertainty contributions in percent (%) to the SFR MA burner β_{eff}.

In sodium reactors, the void worth $\Delta\rho_v$ is another important parameter for every transient inducing an increase of the fuel cladding temperature. Its uncertainty was assessed to 46 pcm, 71 pcm and 73 pcm — i.e. 11%, 6% and 22% — respectively when were voided only the inner fuel region, only the outer fuel region and both fuel regions plus the upper sodium plenum. The uncertainty contributions of each single isotopes to the void worth for each of the three cases are reported in Table VII.

	inner	outer	extended
^{23}Na	5.53	9.77	18.66
^{56}Fe	0.77	0.65	2.27
^{238}U	2.78	4.46	12.21
^{239}Pu	1.16	1.87	0.97
^{241}Am	0.48	1.33	0.70
^{243}Am	0.41	0.52	1.10

TABLE VII. Uncertainty contributions in percent (%) to the SFR MA burner void worth. Results are reported for a voiding of only the inner fuel region (inner), only the outer fuel region (outer) and both fuel regions plus the upper sodium plenum (extended).

The Doppler effect was assessed as a reactivity worth of $\Delta\rho_d = -45$ pcm between the reference fuel temperature of 1500 K and 2500 K. The uncertainty was found to be of 6 pcm. Then, the uncertainty contributions of several isotopes were plotted in Table VIII.

^{23}Na	^{56}Fe	^{238}U	^{239}Pu	^{241}Am	^{243}Am
1.11	7.60	8.55	2.24	0.93	4.52

TABLE VIII. Uncertainty contributions in percent (%) to the SFR MA burner Doppler effect assessed as a reactivity worth.

4. Uncertainties on damage metrics

Tungsten is amongst the candidates for plasma-facing material and divertor in fusion setups, therefore a correct quantification of the damage induced on it by fast neutron fluxes is necessary to ensure the durability and commercial relevance of the material. Since the irradiation facilities with fusion-relevant spectra exhibit too low fluxes to achieve any reasonable dose for material qualification, neutron irradiation tests usually take place in fission reactors with fast neutron spectra.

The multi-purpose irradiation facility MYRRHA [7], conceived as an accelerator driven system (ADS), is designed to achieve significant fast neutron fluxes in the spallation target, where material samples can be irradiated for fusion demonstrations. When MYRRHA is operated in subcritical mode, its linear accelerator provides high energy protons that are used in the spallation target to create neutrons and sustain the fission chain. Then, the reactor configuration allows the production of neutron fluxes up to several hundreds of MeV (Figure 9).

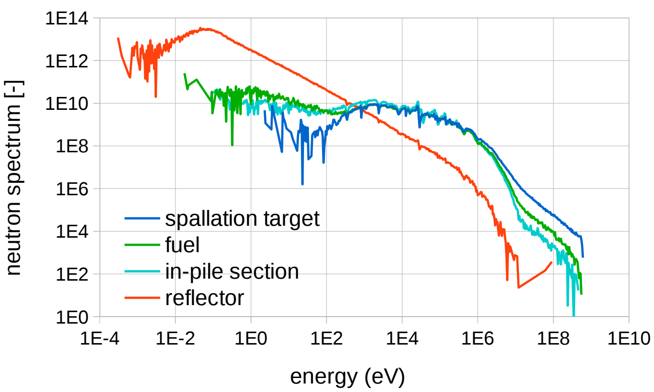

Fig. 9. Average neutron spectra (in relative units) in four locations of the MYRRHA subcritical core.

In this section, dpa (displacements per atom) and associated uncertainties were calculated for ^{184}W simulating MYRRHA's irradiating conditions in the spallation target. The displacement cross sections were calculated with the NJOY module HEATR [11] and nuclear data from ENDF/B-VII.1 [10] and TENDL-2015 [16]. JEFF-3.2 [17] was not included in the comparison as its ^{184}W displacement cross section presents an inconsistency above 30 MeV, which derives from a incorrect estimate of the ^{182}Ta production yield. Uncertainties on cross sections (MF=33) and angular distributions (MF=34) were propagated using SANDY. A plot of the displacement cross sections and their uncertainties calculated with SANDY is reported in Figure 10.

Then, dpa were evaluated using the NRT model [18]. The dpa per year values and uncertainties for ^{184}W were calculated and reported in Table IX.

Dpa uncertainties from ENDF/B-VII.1 underestimate TENDL-2015 results. Moreover, the dpa uncertainty contribution coming from displacement cross sections above 20 MeV appears to be too low (< 1%), although the contribution to the dpa values is still larger than 15%. The lack of nuclear data uncertainties at such energies, where neutrons produce the largest damage, is a major fault when dealing with irradiation facilities such as MYRRHA, where the neutron flux above 20 MeV is still significant.

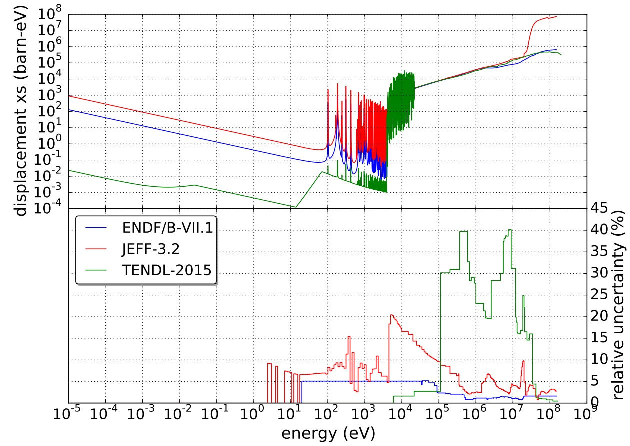

Fig. 10. Displacement cross sections and relative uncertainties of ^{184}W.

	ENDF/B-VII.1	TENDL-2015
dpa/y	11.31 ± 0.08	11.59 ± 2.35
fraction above 20 MeV (%)	16.94	15.96
fraction of variance above 20 MeV (%)	0.10	0.00

TABLE IX. Dpa and uncertainty values for ^{184}W subject to the neutron flux in the MYRRHA spallation target (2.98×10^{15} n/cm^2/s).

IV. CONCLUSIONS

A Monte Carlo sampling code called SANDY for the uncertainty propagation of nuclear data was proposed. SANDY can propagate any nuclear data covariance available in ENDF-6 files. Thanks to its variance decomposition capabilities, SANDY can also identify which input parameter, or group of parameters, produces the largest response uncertainty. SANDY was effectively tested against four test cases related to fast reactor applications. Uncertainties were quantified on multiple responses such as integrated cross sections over energy, k_∞, k_{eff}, β_{eff}, reactivity worths and dpa. Also SANDY was not limited by the choice of the solver and of the model, as several nuclear codes and non-linear models were studied. We propose SANDY as a complete and consistent method to propagate nuclear data uncertainties for nuclear studies.

Several issues on the existing covariance matrices were found. Amongst them, we report the large uncertainty associated to the ^{235}U radiative capture cross section — i.e. larger than 35% — in the energy range of few keV. Such data produced a huge uncertainty contribution to the k_∞ calculation for the VENUS-F reactor, which is loaded with 30 wt.% enriched uranium.

The uncertainty propagation in ASTRID loaded with a large fraction of minor actinides showed that the minor actinides' evaluated uncertainty data are not negligible for several responses. Still they fall behind the ^{238}U data, which always produce the largest uncertainties.

Eventually, in the calculation of dpa uncertainties, a general lack of covariance data was found in several nuclear data libraries for cross sections at energies beyond a few MeV. This lack could pose a problem for the damage metrics uncertainty quantification in system such as MYRRHA, where a significant part of the neutron spectra exceeds these energies.

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