

UNCERTAINTY QUANTIFICATION IN FRENETIC CALCULATIONS OF ALFRED LEAD-COOLED FAST REACTOR

Nicolò Abrate¹, Sandra Dulla¹, and Piero Ravetto¹

¹Politecnico di Torino, Dipartimento Energia, NEMO group

Corso Duca degli Abruzzi, 24 - 10129 Torino (Italy)

nicolo.abrate@polito.it, sandra.dulla@polito.it, piero.ravetto@polito.it

ABSTRACT

The paper shows the application of the most recent sensitivity techniques implemented in Serpent-2 in order to propagate the uncertainty from the nuclear data to the macroscopic, homogenised cross sections of the ALFRED reactor, which is then simulated with the multi-physics code FRENETIC. The main results are encouraging and define a possible methodology to propagate the nuclear data uncertainties to the main macroscopic parameters computed with FRENETIC, in order to perform thorough safety analyses for the ALFRED reactor.

KEYWORDS: lead fast reactor; nuclear data; sampling; uncertainty propagation; multi-physics codes

1. INTRODUCTION

One of the most important phases in the safety assessment of a nuclear reactor design is related to the quantification of the major uncertainties that can affect the operational conditions of the plant. As far as the neutronic design is concerned, there are mainly two kinds of uncertainty sources: on one side, the approximations introduced by the physico-mathematical model (e.g., multi-group vs. continuous-energy, diffusion vs. transport, ...), on the other the uncertainties associated to the model input data, i.e. the geometrical parameters, the operating conditions, the experimental nuclear data, and so on.

The reference model in reactor physics is indeed the transport equation, and the reference computational tool to solve it is the Monte Carlo (MC) method, since it is able to cover the whole phase space without any discretisation, provided that the statistical samples are large enough. Nevertheless, practical applications, especially when design- and safety-related, require fast yet reliable tools like multi-group diffusion codes. In order to fairly reproduce the reference results, these tools need suitable energy-collapsed and space-homogenised material constants that are usually prepared using fine-group deterministic codes like the ECCO-ERANOS system [1] or, more recently, using detailed stochastic transport that read continuous-energy data from the nuclear data libraries. Therefore, in order to correctly quantify the impact of the nuclear data uncertainties on the chain calculation output, propagating them through the deterministic or MC simulation to the multi-group constants is extremely relevant, although quite computationally expensive.

Thanks to the recent developments in the Serpent-2 MC code [2], there are nowadays two ways of performing the Sensitivity Analysis (SA) needed for a first-order Uncertainty Quantification (UQ):

the Generalized Perturbation Theory (GPT) and the eXtended Generalized Perturbation Theory (xGPT) [3]. While the first one is common also to the deterministic codes, xGPT is peculiar of stochastic transport since it allows to exploit the continuous-energy projected coefficients. A recent uncertainty propagation study performed for the Molten Salt Fast Reactor (MSFR)[4] highlighted some difficulties arising in the study of homogenized multi-group constants, due to the intrinsic necessity to perform full-core simulations for a MSR, leading to an impracticable computational cost to reach statistical convergent results.

Nevertheless, the application of these methods should be interesting also for other GEN-IV reactor design, such as Lead-cooled Fast Reactors (LFR), as the heterogeneous arrangement of the core assemblies would allow to focus the attention on a specific region, thus reducing the computational burden. Therefore, the primary objective of this work is to prove the feasibility of the MC propagation of the uncertainty from the basic nuclear data to the multi-group constant for a LFR design. As a second step, the uncertainty is then propagated to two relevant integral quantities, i.e. k_{eff} and the assembly power P_{ASS_i} , that are evaluated with the multiphysics code FRENETIC (Fast REactor NEutronics/ThermohydraulicS), developed at Politecnico di Torino in the last years [5].

The liquid metal fast reactor design chosen for this analysis is the EU LFR demonstrator, the ALFRED reactor [6]. The results presented in this work should define a possible methodology to propagate uncertainty from basic nuclear data to macroscopic output quantities using FRENETIC, establishing a procedure to be applied extensively to perform uncertainty quantification studies for LFRs.

2. UNCERTAINTY QUANTIFICATION TECHNIQUES EMPLOYED

Uncertainty Quantification techniques are basically divided into two categories: direct sampling and surrogate techniques. The first one, employed, for example, in the so-called Total Monte Carlo method (TMC) [7], is very accurate and does not suffer from the curse of dimensionality, allowing thus to assess the impact of many parameters at the same time. However, the main limit of such approach is that it is extremely time consuming, as it converges as a $1/\sqrt{N}$, where N is the number of samples. Therefore, practical studies usually employ surrogate, approximated models, like the first-order sandwich formula [8],

$$\text{var}[R] = \vec{S}_x^R \text{cov}[\vec{x}] \vec{S}_x^{R^T}, \quad (1)$$

where var stands for the variance of a certain response R , S is the sensitivity of R to a variation in the input x , and cov is the covariance matrix of the input.

In nuclear data uncertainty quantification, the UQ is traditionally performed employing equation (1), since the covariance of the input can be evaluated on a multi-group structure taking the appropriate subsection in the nuclear data ENDF-6 format files and processing it with nuclear data codes like NJOY [9], while the group-wise sensitivity coefficients are estimated with well-established techniques like the already mentioned GPT, usually available both in deterministic and stochastic codes, although in the latter case the number of energy groups has to be limited because of statistical reasons. GPT can provide a first-order estimate of the sensitivity coefficient of the perturbed reaction rates. To overcome this limit and to fully exploit the continuous-energy capabilities of stochastic transport, it is possible to employ the xGPT method, which allows to retrieve S as a projection on basis functions b_{Σ_i} extracted from a continuous-energy covariance matrix. When a set

of perturbed data evaluations is available, xGPT can work in a TMC-like way, combining the projected coefficients $S_{b_{\Sigma_i}}$ and the input random responses to build a surrogate response distribution. Unfortunately, it is not possible to extract the continuous-energy covariance information directly from the data with the current processing codes. The only possible workaround is to exploit the T6 package [10], which is a collection of codes able to produce continuous-energy random nuclear data files. If a sufficiently large set of perturbed data was generated, the continuous-energy covariance matrix could be then extracted from the data themselves. The main drawback of such procedure is that the random evaluations are extremely computationally intensive. Therefore, the construction of a set of ^{239}Pu random evaluations for this work with T6 is still ongoing.

In order to exploit the TMC-like capability of xGPT, the interest in having a set of perturbed nuclear data is strong. To build this set with a good compromise in terms of both cost and accuracy, the approach recently tested on the MSFR in the framework of the European Project SAMOFAR [4] can be employed. This methodology consists in generating the covariance matrix on a fine-group mesh, using the SAMpler of Nuclear Data and uncertainty (SANDY) code [11], which takes as input the covariance section of the ENDF-6 file elaborated by the ERRORR module of NJOY and produces a set of random evaluations. It must be remarked here that since SANDY is only devoted to random sampling and reads the covariance as an input, it can produce the data in a much faster way than T6, that builds each each single evaluation from scratch using nuclear physics models. Figure 1 shows the comparison between the correlation matrices of ^{239}Pu evaluated with

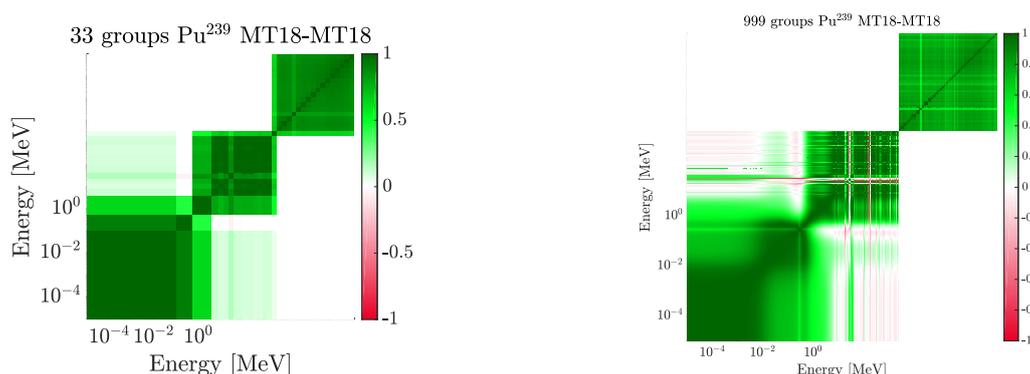


Figure 1: *ECCO 33-groups correlation matrices for MT18 (left) and corresponding equally lethargy spaced 999 groups correlation matrices (right).*

the ECCO-33 energy grid and the corresponding matrices scored on a grid of 999 points equally spaced along the lethargy axes.

3. NUCLIDE SELECTION AND ALFRED MODEL

Thanks to the past experience related to the MSFR, also in this case the choice of the nuclide for the UQ study involved a fissile species, the ^{239}Pu . The main reasons for this choice are its abundance and its impact on the fission process, which is expected to be quite significant. In order to limit the UQ analysis, the only macroscopic cross section considered for the uncertainty propagation is the multi-group macroscopic fission cross section of the fuel assembly, Σ_f , as one of

Table 1: Six-group data adopted to perform the macroscopic cross section energy collapsing and spatial homogenisation [12].

Group	Upper boundary [MeV]	Lower boundary [MeV]
1	$2.000 \cdot 10^1$	$1.353 \cdot 10^0$
2	$1.353 \cdot 10^0$	$1.832 \cdot 10^1$
3	$1.832 \cdot 10^{-1}$	$6.738 \cdot 10^{-2}$
4	$6.738 \cdot 10^{-2}$	$9.119 \cdot 10^{-3}$
5	$9.119 \cdot 10^{-3}$	$2.000 \cdot 10^{-5}$
6	$2.000 \cdot 10^{-5}$	$1.000 \cdot 10^{-11}$

the most influenced by the selected nuclide. The reference thermodynamic condition considered for the study is uniform temperature of 673 K for the whole system. In order to avoid missing covariance or MT data, the ^{239}Pu file present in the JEFF-3.1.1 library, that we usually employ for our calculations, is substituted with one coming from the latest ENDF-B/VIII release. This choice provides also consistency for the generation of the ^{239}Pu random evaluations with T6, which takes some data from ENDF-B/VIII. Thanks again to the past experience with the UQ performed at

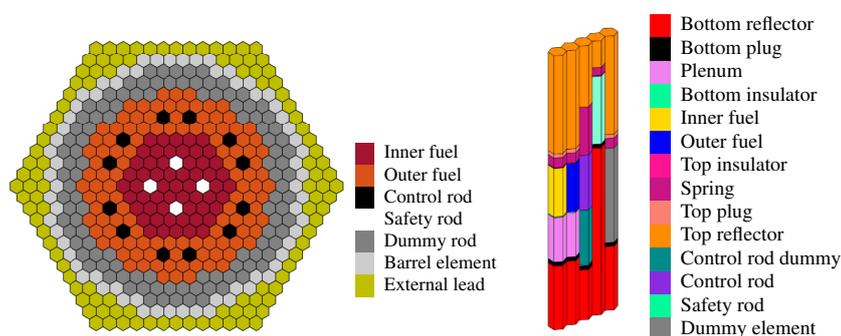


Figure 2: Radial (left) and axial (right) sections of ALFRED 3D model.

3D full-core level, we take advantage of the heterogeneous arrangement of the core to focus our analysis on a specific kind of assemblies, in order to reduce the computational domain (and thus the burden) and, at the same time, to increase the Monte Carlo simulation level of detail. Therefore, to estimate the influence of ^{239}Pu nuclear data on the six-group (the energy grid is given in Table 1) homogenised fission macroscopic cross section, which is then used in FRENETIC, the 3D full-core Serpent-2 model (see figure 2) employed for the generation of the cross sections for FRENETIC is simplified to a radially infinite system made of 60 cm inner fuel assemblies, axially surrounded by the top and bottom reflectors. This model certainly yields less accurate inner fuel cross sections with respect to the ones obtained with the full-core model, but allows to increase the statistics related to the sensitivity coefficients estimation.

4. UNCERTAINTY QUANTIFICATION RESULTS

In this section, we briefly summarize the main results of our analysis.

4.1. GPT results

Since the group-wise sensitivity coefficients estimated with GPT approach provide a very clear picture of the physics and can provide a comparison term for the xGPT, a first calculation employing this approach is performed scoring the sensitivities on the ECCO-33 energy grid. The simulation is run with about $2 \cdot 10^9$ active particles and 10 latent generations on 240 CPUs (Intel(R) Xeon(R) CPU E5-2680 v3 @ 2.50GHz) for a total time of almost 16 hours. Figure 3 shows the behaviour of

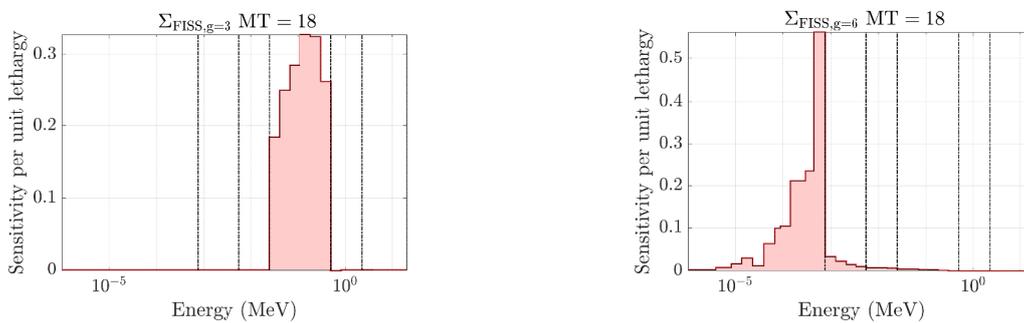


Figure 3: *ECCO 33-groups sensitivity coefficients evaluated with GPT technique.*

the relative sensitivity coefficients of the macroscopic fission cross section for two energy groups. It is interesting to notice that $\Sigma_{f,6}$ is slightly sensitive also to perturbations on the two adjacent upper groups, while Σ_f in groups from 1 to 5 only depends on what occurs inside each group (only $\Sigma_{f,3}$ is shown for sake of brevity). The sensitivity coefficients for MT18 (fission) and MT102 (radiative capture) are then combined with the corresponding ECCO-33 covariance matrix in order to retrieve the total uncertainties, as reported in Table 2.

Table 2: Values computed by GPT and percentage relative standard deviations due to the uncertainties in MT18-MT102 reactions for Pu-239.

Parameter	Value	% Nuclear data uncertainty
$\Sigma_{f,1}$	0.006894 ± 0.000021	2.34938 ± 0.000150
$\Sigma_{f,2}$	0.003072 ± 0.000015	1.23322 ± 0.000061
$\Sigma_{f,3}$	0.001799 ± 0.000005	1.01492 ± 0.000032
$\Sigma_{f,4}$	0.002213 ± 0.000010	1.02758 ± 0.000016
$\Sigma_{f,5}$	0.004146 ± 0.000020	0.69354 ± 0.000066
$\Sigma_{f,6}$	0.013459 ± 0.000083	0.34228 ± 0.000180

4.2. xGPT results

The same case of the previous section is run in xGPT mode with about $2 \cdot 10^9$ active particles and 10 latent generations on 240 CPUs (Intel(R) Xeon(R) CPU E5-2680 v3 @ 2.50GHz) for a total time of almost 40 hours. The projected sensitivities $S_{b_{\Sigma_i}}$ are evaluated using 35 basis functions approximating the ^{239}Pu sample covariance matrix with an error less than 0.01% [4]. The sample covariance matrix is extracted from the random evaluations generated by SANDY. Figure 4 provides some visual representations of the values of the Σ_f sensitivity coefficients to

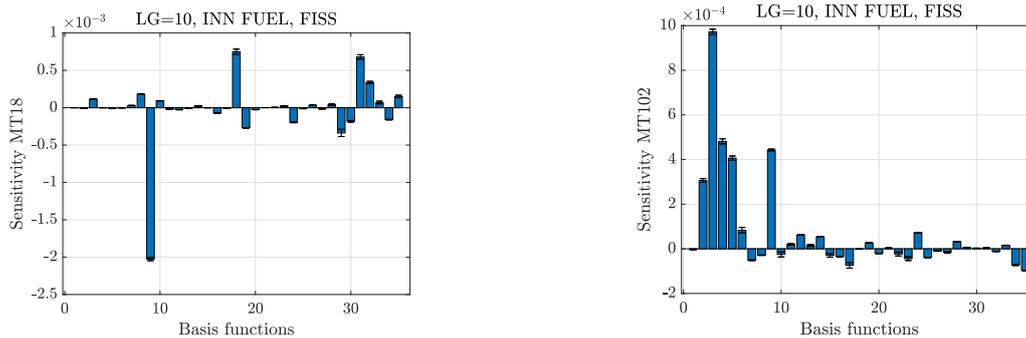


Figure 4: *Projected sensitivity coefficients evaluated with xGPT technique for MT18 and MT102.*

each basis functions of MT18 and MT102 for the same energy bin, corresponding to the first group. The physical interpretation of these sensitivity coefficients is more complicated with respect to the previous GPT case.

Table 3: Values computed by xGPT and percentage relative standard deviations due to the uncertainties in MT18-MT102 reactions for Pu-239.

Parameter	Value	% Nuclear data uncertainty
$\Sigma_{f,1}$	0.006894 ± 0.000021	0.41276 ± 0.000065
$\Sigma_{f,2}$	0.003072 ± 0.000012	0.15817 ± 0.000210
$\Sigma_{f,3}$	0.001799 ± 0.000005	0.00488 ± 0.001300
$\Sigma_{f,4}$	0.002213 ± 0.000010	0.01191 ± 0.003000
$\Sigma_{f,5}$	0.004146 ± 0.000020	0.01239 ± 0.003100
$\Sigma_{f,6}$	0.013459 ± 0.000083	0.00006 ± 0.025000

Table 3 shows the relative percentage uncertainties related to Σ_f in each group. With respect to the previous case, the values are here quite difficult to be interpreted. The inspection of the statistical error associated to the computed uncertainties would suggest that the statistics is not good enough in this case, meaning that more accurate simulations need to be performed.

Table 4: Relative sensitivity coefficients for k , power in central assembly P_1 and power in a peripheral assembly P_5 with respect to Σ_f in the various groups adopted, estimated directly with FRENETIC.

Parameter	Value	Parameter	Value	Parameter	Value
$S_{\Sigma_f,1}^k$	$9.7451 \cdot 10^{-2}$	$S_{\Sigma_f,1}^{P_1}$	$5.3879 \cdot 10^{-1}$	$S_{\Sigma_f,1}^{P_5}$	$1.5713 \cdot 10^{-1}$
$S_{\Sigma_f,2}^k$	$1.6296 \cdot 10^{-1}$	$S_{\Sigma_f,1}^{P_1}$	$8.7135 \cdot 10^{-1}$	$S_{\Sigma_f,1}^{P_5}$	$2.9395 \cdot 10^{-1}$
$S_{\Sigma_f,3}^k$	$1.8971 \cdot 10^{-1}$	$S_{\Sigma_f,1}^{P_1}$	$1.2022 \cdot 10^{+0}$	$S_{\Sigma_f,1}^{P_5}$	$2.2454 \cdot 10^{-1}$
$S_{\Sigma_f,4}^k$	$6.6389 \cdot 10^{-2}$	$S_{\Sigma_f,1}^{P_1}$	$3.7455 \cdot 10^{-1}$	$S_{\Sigma_f,1}^{P_5}$	$1.1383 \cdot 10^{-1}$
$S_{\Sigma_f,5}^k$	$5.3438 \cdot 10^{-2}$	$S_{\Sigma_f,1}^{P_1}$	$3.1380 \cdot 10^{-1}$	$S_{\Sigma_f,1}^{P_5}$	$8.5262 \cdot 10^{-2}$
$S_{\Sigma_f,6}^k$	$1.0700 \cdot 10^{-2}$	$S_{\Sigma_f,1}^{P_1}$	$7.0228 \cdot 10^{-2}$	$S_{\Sigma_f,1}^{P_5}$	$8.7047 \cdot 10^{-3}$

5. FRENETIC sensitivity coefficient calculation

After the propagation of the nuclear uncertainty to the Σ_f parameter, the second step of the work consists in estimating the sensitivity of some macroscopic responses to the perturbations of the fission homogenised cross sections characterising the inner fuel assemblies of ALFRED. To perform this task, we employed FRENETIC, a multiphysics code that adopts a 1D advection/diffusion model in the thermo-hydraulics module and a multi-group nodal diffusion model for neutronics. As a starting point, the code is employed to perform standalone neutronic calculations for a direct estimation of the sensitivity coefficients as

$$S_{\Sigma_f}^R = \frac{\delta R/R}{\delta \Sigma_f/\Sigma_f} = \frac{(R_{ref} - R_{pert})/R}{(\Sigma_{f,ref} - \Sigma_{f,pert})/\Sigma_f}, \quad (2)$$

where R is one of the selected responses: the effective multiplication parameter, the power in the central assembly, and the power in one of the peripheral inner fuel assembly (for the correct identification of the region, please refer to Figure 2). The value of the $\delta \Sigma_f$ is computed assuming variations of 0.1%, -0.1%, 0.2% and -0.2% separately for each group, in order to verify that the linear assumption for this variation is satisfied. Since the coupled simulation would require a complete set of temperature-dependent multi-group constants for the thermal feedback calculations and, therefore, also a complete set of perturbations for each temperature, the coefficients are estimated assuming a steady-state uniform temperature distribution in the core. The values of the sensitivity coefficients computed as described above are listed in table 4.

Combining the sensitivities computed directly by FRENETIC with the Σ_f uncertainties computed via GPT per each response, the resulting average values and relative uncertainties are $1.12194 \pm 3.686 \cdot 10^{+2}$ [pcm] for k , 2.691219 [MW] ± 2.1075 % for the power in the central assembly and 2.240166 [MW] ± 0.5804 % for the power in the peripheral assembly.

6. CONCLUSIONS

The latest Serpent-2 sensitivity calculation capabilities are applied to propagate the uncertainty from the MT18-MT102 reactions of ^{239}Pu to the macroscopic, multi-group fission cross section of the ALFRED inner fuel assembly type. The resulting uncertainty is then propagated to the main neutronic macroscopic parameters computed by the multiphysics code FRENETIC. The results of the calculations are encouraging, in spite of the fact that xGPT results need some more investigation. In addition to this aspect, also the propagation of the uncertainties through a fully coupled neutronics/thermo-hydraulics calculations deserves to be tested, in order to link nuclear data uncertainties to the main thermo-hydraulics parameters.

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REFERENCES

- [1] G. Rimpault, D. Plisson, J. Tommasi, R. Jacqmin, D. Verrier, and D. Biron. The ERANOS Code and Data System for Fast Reactor Neutronic Analyses. *Physor 2002*, (November), 2002.
- [2] J. Leppänen, M. Pusa, T. Viitanen, V. Valtavirta, and Toni Kaltiaisenaho. The Serpent Monte Carlo code: Status, development and applications in 2013. *Annals of Nuclear Energy*, 82:142–150, 2015.
- [3] M. Aufiero, M. Martin, and M. Fratoni. xGPT: Extending Monte Carlo Generalized Perturbation Theory capabilities to continuous-energy sensitivity functions. *Annals of Nuclear Energy*, 96:295–306, 2016.
- [4] N. Abrate, M. Aufiero, S. Dulla, and L. Fiorito. Nuclear Data Uncertainty Quantification in Molten Salt Reactors with xGPT. In *Proceedings of the ANS International Conference M&C2019*, Portland, OR, August 25-29 2019.
- [5] R. Bonifetto, S. Dulla, P. Ravetto, L. Savoldi Richard, and R. Zanino. A full-core coupled neutronic/thermal-hydraulic code for the modeling of lead-cooled nuclear fast reactors. *Nuclear Engineering and Design*, 261:85–94, aug 2013.
- [6] G. Grasso, C. Petrovich, D. Mattioli, C. Artioli, P. Sciora, D. Gugiu, G. Bandini, E. Bubelis, and K. Mikityuk. The core design of ALFRED, a demonstrator for the European lead-cooled reactors. *Nuclear Engineering and Design*, 278:287–301, 2014.
- [7] D. Rochman, A. J. Koning, S. C. Van Der Marck, A. Hogenbirk, and C. M. Sciolla. Nuclear data uncertainty propagation: Perturbation vs. Monte Carlo. *Annals of Nuclear Energy*, 38(5):942–952, 2011.
- [8] Dan G Cacuci. *Sensitivity & Uncertainty Analysis, Volume I: Theory*. CRC Press, Boca Raton, 2003.
- [9] R E Macfarlane, Contributing Authors, D W Muir, R M Boicourt, A C Kahler, J L Conlin, and W Haeck. The NJOY Nuclear Data Processing System, Version 2016. Technical report, 2018.
- [10] D. Rochman, A.J. Koning, J.Ch. Sublet, M. Fleming, E. Bauge, S. Hilaire, P. Romain, B. Morillon, H. Duarte, S. Goriely, S.C. van der Marck, H. Sjöstrand, S. Pomp, N. Dzysiuk, O. Cabellos, H. Ferroukhi, and A. Vasiliev. The TENDL library: Hope, reality and future. *EPJ Web of Conferences*, 146:02006, 2017.
- [11] L. Fiorito, G. Žerovnik, A. Stankovskiy, G. Van den Eynde, and P. E. Labeau. Nuclear data uncertainty propagation to integral responses using SANDY. *Annals of Nuclear Energy*, 101:359–366, 2017.
- [12] G F Nallo, N Abrate, S Dulla, Ravetto P., and Valerio D. Neutronic benchmark of the FRENETIC code for the multiphysics analysis of lead fast reactors. *The European Physical Journal Plus*, 123, 2020.