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A weight window approach for dose rate calculations in Lead-cooled Fast Reactors with OpenMC

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Abstract. This paper presents the application of a variance reduction technique for radiation shielding calculations in Lead-cooled Fast Reactors (LFRs) using the OpenMC Monte Carlo code. The study focuses on assessing the computational efficiency of the Method of Automatic Generation of Importances by Calculation (MAGIC). This technique is employed to generate weight windows for Monte Carlo simulations, aiming at enhancing the efficiency of dose rate estimations for LFRs. Through a detailed study of a LFR mock-up model, the performance differences between a MAGIC-accelerated and a non-accelerated simulation are investigated in terms of both accuracy and computational cost. The results demonstrate the benefits of the variance reduction method, showing its effectiveness in spreading particles throughout the model while improving the accuracy of Monte Carlo estimates far from the core. In addition, this work demonstrates the performances of the MAGIC method in eigenvalue calculations. This work shows an interesting optimisation of Monte Carlo simulations for LFRs and can be considered as a first milestone for *new*cleo's radiation shielding studies.

1 Introduction

Lead-cooled Fast Reactors (LFRs) are one of the most promising and mature Gen-IV concepts. Their main features encompass a fast neutron spectrum and the adoption of liquid lead as a coolant. The unique neutronic characteristics of lead, such as its diffusive properties and low absorption cross-section, make it an attractive choice for enhancing reactor safety and efficiency. As LFRs gain prominence in the future nuclear energy landscape, it becomes imperative to thoroughly investigate and optimise various aspects of their operation, including radiation protection calculations.

During the conceptual design phase of a nuclear reactor unit, emphasis must be placed on dose rate assessment. In particular, the estimation of the dose rate on the vessel roof is of paramount importance for verifying the feasibility of *in-situ* interventions during reactor operation and maintenance.

Lead is very effective at shielding gamma radiation. However, neutrons readily penetrate lead due to the low absorption and high elastic scattering cross sections. Therefore, without

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proper shielding, a large fraction of the neutrons can escape from the core and cause the emission of secondary photons through interaction with structures.

The assessment of the dose rate at the top of the reactor pool requires the calculation of photon and neutron fluxes that are several orders of magnitude smaller than those inside the core. Hence, the well-known issues of classical deep-penetration problems in the Monte Carlo (MC) framework arise. In addition to the slow convergence rate of the MC method, which scales as $1/\sqrt{N}$, where N indicates the number of particle histories, the major challenge is the very small number of particles reaching the tallying volumes far from the source. Hence, a standard simulation would require an extensive computational time and, in certain cases, may not even be possible.

These problems are usually overcome by using Variance Reduction (VR) techniques, i.e. methods capable of artificially increasing the probability of rare events, while maintaining the same expected value. Among these, Global Variance Reduction (GVR) methods aim at equally populating each region of the model, thus allowing physical observables to be estimated with an acceptable accuracy across the entire model [1]. By providing global information, and highlighting possible preferential propagation channels for radiation, this class of variance reduction methods is of considerable interest since the preliminary design stages of nuclear power plants.

The Weight Window (WW) is a popular VR method that allows control of the particle population by selectively splitting or subjecting particles to Russian roulette, depending on their likelihood of contributing to a given score [2]. Weight windows are defined on a spatial and energy mesh of the entire phase space. For each of these phase space regions, a weight window consists of a range of statistical weights within which the particle is allowed to remain. If its weight is greater than the WW upper bound, it is split, whereas if the weight is less than the lower bound, it plays Russian roulette.

This paper presents an application of a WW generation methodology known as Method of Automatic Generation of Importances by Calculation (MAGIC) [3, 4]. This approach allows to get an efficient calculation of the WW parameters for the calculation of the neutron and photon fluxes throughout the model. MAGIC is used to compute the dose rates delivered on the reactor roof for the case of a simple yet representative mock-up model of a LFR reactor, using the OpenMC Monte Carlo code [5]. The comparison between non-accelerated simulations and simulations using the MAGIC method will be evaluated in terms of a proper Figure of Merit. In addition, the consistency between the two sets of results will be verified.

The MAGIC method has been preferred to adjoint-based techniques, such as the FW-CADIS [1], due to its simplicity in setup and ready availability in OpenMC. Furthermore, the generation of importance functions by means of deterministic adjoint calculations might be problematic due to convergence issues of deterministic codes in the presence of highly-diffusive material.

All calculations presented and discussed in the present document have been generated using OpenMC, version 0.13.3, and a stand-alone version of the MAGIC weight window generator [6].

2 Methodology

In this section, the methodology followed to tackle the deep penetration problem is presented and discussed.

2.1 The Weight Window Method

The objective of a variance reduction method consists of artificially increasing the particle population in the most "important" regions of the model by splitting the particles that are more likely to contribute to the response of interest and killing those that are less likely. A WW-based variance reduction method requires a spatial and energy discretization of the phase space. For each phase-space region, the weight window is defined as the interval of admissible statistical weights, comprised between an upper and a lower bounds, w_u and w_l respectively. Whenever a particle collides in a given phase-space region, its weight w is compared with the weight window of the region. If the weight of the particle is larger than w_u, the particle is split into N particles of weight w/N, where

$$N = \min\{N_{max}, \lceil w/w_u \rceil\}, \tag{1}$$

and N_{max} is the maximum number of splits. If the weight of a particle falls below w_l, Russian Roulette is played. Two additional controls are also operated in OpenMC. The code allows to limit the maximum number of splittings events per particle history and to set a minimum allowable particle weight. OpenMC has a built-in weight window capability [7], which allows the assignment of a lower and upper bound map to the model settings in the form of a matrix.

2.2 The MAGIC method

The OpenMC WW maps can be generated using the `openmc_weight_window_generator` python module, which implements the MAGIC (Method of Automatic Generation of Importances by Calculation) method [3]. The cornerstone idea of this approach is to use the scores of low-accuracy simulations to iteratively improve the WW parameters. A first calculation is carried out either in continuous-energy mode or using the multi-group approximation, simulating a relatively low number of particle histories. The goal of this first simulation is to estimate the flux over a phase space discretization, defined by the Cartesian product of a 3D spatial mesh enveloping the entire reactor geometry and a user-defined energy grid. For each of these meshes, the weight window upper and lower bounds are calculated based on the flux score from the previous MC calculation. The process is repeated until the weight window accuracy is judged satisfactory. The calculation route ends with an accurate Monte Carlo simulation, providing the estimations that are required by the radiation shielding study.

At each iteration, the `openmc.weight_window_generator` function receives as input the flux tally results. For each energy bin g, and for each spatial region i of the mesh, the WW lower bound $w_{l,i,g}$ is set equal to

$$w_{l,i,g} = \phi_{i,g} / \max\{\phi_{i,g} : i = 1, N_i\} \quad g = 1, N_g,\ i = 1, N_i, \tag{2}$$

where $\phi_{i,g}$ is the value of the integral of the flux in the phase space region i, g. The upper bound values are generated by multiplying the lower bounds by a constant, which is set to 5 by default [8]. The WW is deactivated in the phase space regions where either the expected value of the flux is zero, or its relative standard deviation is larger than a used-defined cut-off parameter. The lower and upper bound weights in each phase space region constitute the WW map. Such a map is then provided to the successive MC calculation.

2.3 Welch's T-Test

The fundamental requirement for any variance reduction method is providing an unbiased sample mean estimation with respect to the standard MC calculation. For a sufficiently large number of particle replica, both sample means are normally distributed, thanks to the Central Limit Theorem. Then, the Welch's T-test can be used to ensure that the calculation with VR is unbiased by comparing the expected values of the corresponding normal distributions. [9]. In the present document, the analysis is applied to the comparison of the flux estimations of the MC calculation with and without WW. The test consists in computing the derived quantity t, which is defined as the ratio

$$t = \frac{|\phi_{ww} - \phi|}{\sqrt{\sigma_{ww}^2 + \sigma^2}}, \tag{3}$$

where ϕ_{ww} and ϕ are the flux estimations with and without WW, while σ_{ww} and σ are their respective standard deviations. If the parameter t is smaller than 3, the two estimates, ϕ_{ww} and ϕ, agree within 3 standard deviations, and the test is passed.

2.4 Figure of Merit (FOM)

The effectiveness of VR methods is generally measured by computing the Figure of Merit of the MC simulation. This is defined as the inverse of the product of the variance σ^2 of a certain MC estimate and the calculation time τ of the active particle histories, i.e.

$$FOM = \frac{1}{\sigma^2 \tau}. \tag{4}$$

Assuming that the convergence of the MC calculation is equal to the ideal one, i.e. the standard deviation $\sigma \propto 1/\sqrt{N}$, and $\tau \propto N$, where N is the number of particle histories, the FOM value is independent of N. Therefore, the ratio between the FOM of the WW simulation (FOM_{ww}) and the FOM of the simulation without WW (FOM), expressed as

$$\Gamma = \frac{\mathrm{FOM}_{ww}}{\mathrm{FOM}}, \tag{5}$$

indicates how faster the former is compared to the latter, provided equal variances.

2.5 Simulation Settings

The settings used for the calculation without WW are shown in Table 1, while Table 2 provides the settings used for the MAGIC iterations and the final MC calculation using WW. The settings used for the MAGIC are displayed in Table 3.

Parameter	**Value**
Number of MPI processes	1
Number of threads per process	48
Number of batches	3000
Number of inactive batches	20
Number of particles per batch	10^6

Table 1: Simulation settings for the Monte Carlo calculation without weight windows.

Parameter	**Value**
Number of MPI processes	1
Number of threads per process	48
Number of batches	100
Number of inactive batches	20
Number of particles per batch	$2 \cdot 10^4$

Table 2: Simulation settings for the Monte Carlo calculation with weight windows.

Parameter	Value
Number of iterations	5
RSD cut-off	0.7
Max splits per splitting event	$1 \cdot 10^6$
Max splits in particle history	$1 \cdot 10^7$
WW upper/lower bound ratio	5

Table 3: MAGIC and weight windows settings.

The MC calculation with WW is characterised by a lower number of particle histories than the one without WW. This is because, with WW, particles histories are much longer due to the large number of particle splits per source particle. Considering two simulations with and without WW, with the same number of batches and particles per batch, the former will actually take longer to complete. All calculations involved in the iterations of the MAGIC method were carried out in continuous-energy and eigenvalue mode, coupling neutron and photon transport. These computations were performed on an almost critical configuration (±30 pcm with respect to the criticality), therefore the fission source is continuously updated through power iterations. The WW were applied to both neutron and secondary photon transport. For the specific reactor model studied in this work, a total number of 5 MAGIC iterations was considered sufficient to guarantee an accurate flux estimation over the whole domain (namely, 5 calculations meant to evaluate the WW maps and one final MC calculation). The MAGIC method was utilised to generate a WW mesh made of $100 \times 100 \times 100$ Cartesian cells with a single energy bin.

All results presented in this work were obtained using the ENDF-B/VIII.0 nuclear data library [10]. Calculations were performed on *new*cleo's HPC cluster mounting Intel Xeon 6336Y CPUs. The calculation of the active batches of the 5 MAGIC iterations took 132 CPU-hours, while the final simulation with WW and the simulation without WW took 61 and 2850 CPU-hours, respectively. The overall duration of the simulation with WW was 193 CPU-hours, comprising the cumulative time taken by the MAGIC iterations and the subsequent final simulation.

3 Description of the LFR Mock-up

The reactor model used in this analysis represents a typical pool-type lead-cooled fast reactor with a MOX-fuelled core and an output thermal power of about 100 MWth. The model is meant to represent the main features of the LFR-AS-30 reactor currently being designed by *new*cleo. The fuel and control assemblies have been homogenised into 2-meter height hexagonal prisms. The dimension of each side of the hexagonal prisms is 20 cm in length. The reactor core consists of a 4-ring hexagonal lattice of fuel assemblies surrounded by 12 control assemblies. The gap between the assemblies is 1 cm.

The core is housed in an AISI-316 steel vessel, which is a straight vertical cylinder closed by two hemispheres. The upper hemisphere has a circular opening leading to a small vertical straight cylinder. The vessel is surrounded by a cylindrical outer vessel, closed at the bottom by a hemisphere.

The reactor vessels are enclosed in a pit made of concrete. The lead free surface is covered with an argon gap, a 20 cm thick layer of borated steel and a 50 cm thick stainless steel roof. The domain consists of a cylinder with a height of 10 m and a diameter of 9 m. All boundaries have vacuum conditions. Figure 1 and Figure 2 show a sketch of the core and a longitudinal section of the reactor model, respectively.

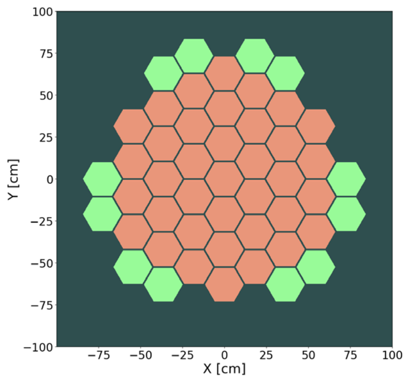

Figure 1: Mock-up model - Reactor core (red: fuel, green: control rods, dark gray: lead).

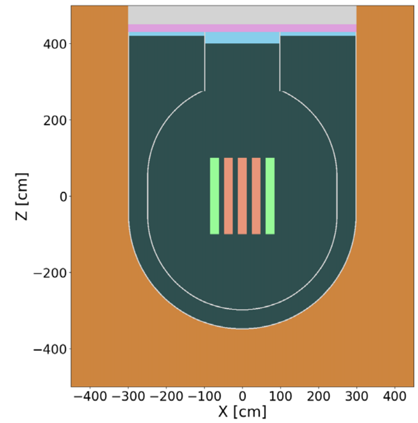

Figure 2: Axial section of the mock-up model (red: fuel, green: control rods, dark gray: lead, light gray: AISI-316, light blue: argon, violet: borated steel, brown: concrete).

This simplified mock-up of the reactor is used here to compare the performances of the MC calculations.

4 Results

The main goal of the MAGIC method is to provide weight windows capable of guaranteeing a score over all the domain within an acceptable accuracy. Therefore, the efficiency of the MAGIC method can be assessed by measuring the ratio of the number of cells in the spatial mesh where the Relative Standard Deviation (RSD) of the neutron flux estimate is lower than a certain threshold, and the total number of mesh cells. Such a ratio, hereafter referred to as the coverage rate, gives an immediate indication of how effective the method is at populating the model with particles, and therefore providing estimations across the whole domain. The coverage rate achieved after 5 consecutive MAGIC iterations is presented in Table 4.

Figure 3 illustrates the estimate of the neutron flux calculated on 50 small volumes placed on the z-axis of the reactor, starting from the bottom of the concrete pit to the top of the vessel roof. Results were obtained from both a weight window accelerated simulation and, whenever possible, a standard simulation. In the following figures, different colours identify different zones in the reactor model, in particular: the concrete pit is depicted in brown, lead in grey, the core in blue, the argon gap in green, the borated steel shielding layer in red, and the AISI-316 vessel roof in yellow. The flux profile shows a steep decrease in structural and shielding materials, such that the standard MC calculation could not provide a flux estimation in these regions.

Similar trends are shown by standard and WW calculations. For each of the tallying volumes where the percentage RSD of the standard simulation is below 20%, the simplified

MAGIC iteration	Coverage RSD<0.2	Coverage RSD<0.5
0	12.00	20.07
1	37.76	43.04
2	59.23	67.25
3	85.58	90.33
4	96.15	97.93
5	98.77	99.89

Table 4: Coverage rate as a function of the number of MAGIC iterations and relative standard deviation.

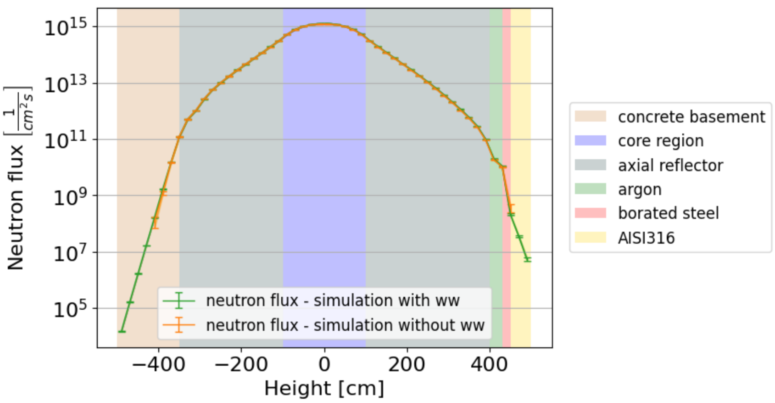

Figure 3: Neutron flux profile along the model vertical axis. Results are displayed together with an error bar corresponding to 1 standard deviation.

Welch's T-test is performed and the FOM is evaluated. Figure 4 displays the results of the Welch's T-test on the neutron flux estimates. It can be noticed how the t value is never larger than 3, proving that the results obtained with the WW method are consistent with those obtained with the standard simulation within 3 standard deviations.

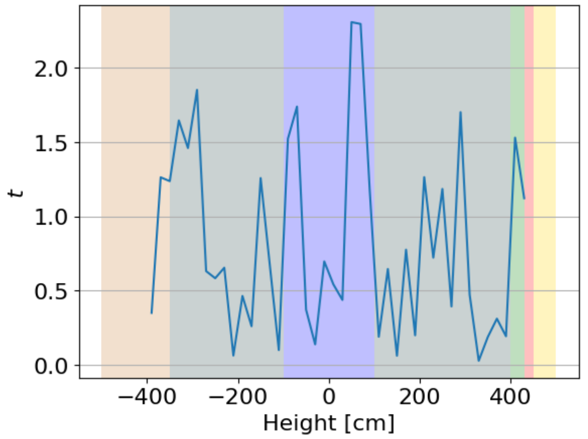

Figure 4: T-test results of neutron flux estimations along the model vertical axis.

However, Figure 4 shows a certain sparsity of t values. The reason for this could be found both in the statistical oscillations introduced by WW, and in the MC power iterations. Since the two MC calculations are criticality calculations, using different numbers of particle per batch, the distribution of the source particles could have a slight influence on the flux estimates.

Figure 5 shows the gain in term of FOM, quantified by Γ, of the simulation using WW with respect to the simulation without WW. For the sake of completeness, dashed lines represent the values of Γ for points featured by a percentage RSD between 20% and 40%. The effectiveness of the MAGIC-WW method is confirmed by Γ values up to 10^3 in the upper part of the reactor and in the reactor pit.

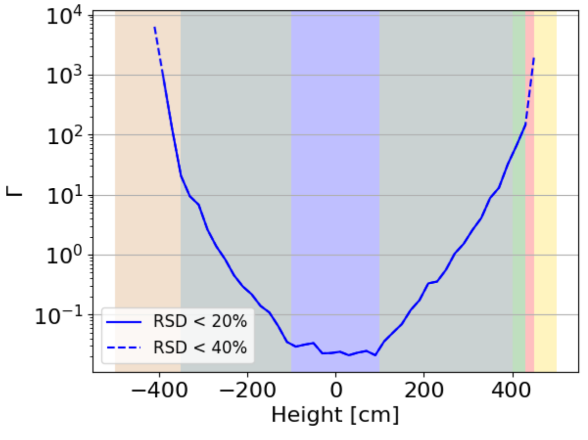

Figure 5: FOM gain of the neutron flux estimation along the model vertical axis.

Figure 6 shows the distribution of the neutron and secondary photon dose equivalent rate [11] along the vertical axis of the reactor system.

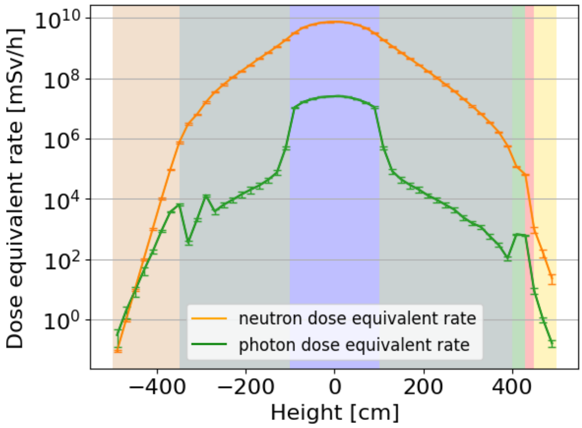

Figure 6: Dose Equivalent rate distribution along the model vertical axis.

The attenuation of the neutron and secondary photon fluxes provided by the lead reactor pool is about four orders of magnitude, while the attenuation caused by the stainless steel roof and the layer of borated steel is more significant. The dose decreases by approximately 9 orders of magnitude from the center of the reactor core to the top of the roof. Such a large flux attenuation demonstrates the need to use variance reduction methods in this class of problems, and at the same time highlights the effectiveness of the MAGIC method.

5 Conclusions and future perspective

This paper shows the application of a variance reduction technique for the radiation protection assessment of LFRs with the Monte Carlo method in a computationally efficient way. Specifically, the objective of the analysis was an accurate estimate of the radiation dose delivered in correspondence of the roof covering the reactor cavity for a mock-up model representative of a typical pool type LFR. The variance reduction methodology adopted for this deep penetration problem is based on weight windows, which are computed using the MAGIC methodology. Compared to other approaches, the adoption of MAGIC does not require external deterministic codes nor modifications to the Monte Carlo code used for the analysis, providing significant ease of use. Thanks to the MAGIC-WW method, the estimation of the unbiased dose rate at the level of the vessel roof was possible within a reasonable time, providing results that would require prohibitive computational resources for a thorough shielding study using a standard, non-accelerated Monte Carlo simulation.

Although already satisfactory, the potential of the MAGIC method could be further explored and improved. The use of an energy mesh with different degrees of refinement should be explored, as well as the use of spatial meshes with variable step sizes depending on the optical thickness featuring the different materials. The use of an adaptive phase space discretisation along with the MAGIC iterations could also be investigated.

References

[1] M. Munk, R. N. Slaybaugh, Nuclear Science and Engineering **193**, 1055-1089 (2019)
[2] Y. Hu, Y. Qiu, U. Fischer, Fusion Engineering and Design **170**, 112551 (2021)

[3] A. Davis, A. Turner, Proceedings of the International Conference on Mathematics and Computational Methods Applied to Nuclear Science and Engineering **M&C 2011**, 112551 (2011)

[4] Yu Zheng et al., Fusion Engineering and Design, **147**, 111238 (2019)

[5] P. K., Romano et al., Annals of Nuclear Energy **82**, 90-97 (2015)

[6] J. Shimwell et al., openmc_weight_window_generator, "https://github.com/fusion-energy/openmc_weight_window_generator" (2022)

[7] Y. Hu, Y. Sha, Y. Qiu, Nuclear Engineering and Technology **54**, 3803-3810 (2022)

[8] T. E. Booth, Genesis of the weight window and the weight window generator in MCNP-a personal history, Tech. Rep. Los Alamos Report LA-UR-06-5807, (2006)

[9] B. L. Welch, Biometrika **34 1-2**, 28-35 (1947)

[10] D.A. Brown et al., Nuclear Data Sheets, 1-142 (2018)

[11] N. Petoussi-Henss et al., Physics in Medicine and Biology **59**, 5209 (2014)