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Optimal choice of free parameters in Monte Carlo burnup simulations

Arman Salehi[a,1], Romain Febvre[a,1]

[a]*KTH Royal Institute of Technology, Division of Nuclear Engineering, AlbaNova University Center, 10691 Stockholm, Sweden*

Abstract

Monte Carlo burnup simulations are computationally very expensive and thus the aim of this paper is to examine the free parameters of a PWR burnup simulations that will produce the optimal cost. The efficiency of a Serpent simulation is affected by parameters such as the length of the time steps and the number of neutron histories simulated. For the purpose of this study, these are manipulated, and the results are presented under the form of a figure of merit. Different schemes can be used to solve various types of burnup problems. Even though it has been observed that the type of scheme does not have a particularly large impact on the results, it has been decided that only one shall be used (J. Dufek and I. Mickus (2020)). Whilst each have their advantages and disadvantages, for this study, the explicit Euler coupling scheme has been designated as the method used for all the simulations. In this technical note, various number of combinations of the free parameters were tested.

Keywords:
Monte Carlo burnup calculations, Time step length, Efficiency, Optimisation.

1. Introduction

Monte Carlo neutron simulations require large amounts of computational power relating to the complexity of the problems. By improving the efficiency of these simulations, they become more practical for research purposes, both in academia and in the industry.

In this study, the optimal computing cost is found by running multiple burnup simulations. Through manipulating the length of the time steps, different ratios of depletion cost to total cost are achieved and a figure of merit (FOM) can be obtained. A longer time step will provide a smaller computation time, but at the price of a lower accuracy. To get the optimal parameters the error must be compared to the computing time.

To ensure the results have no bias, control variables such as the amount of computational power used were implemented.

For this purpose, a 17x17 fuel assembly segment of pure Uranium-235 metal is placed inside a PWR reactor. The coolant used is light water.

The theory behind the explicit Euler coupling method is first examined as well as the figure of merit being explained in Section 2, entitle Theory. In the ensuing section, entitled Results, the outcomes of our simulations are presented under tabular form before being discussed and conclusion drawn from these tests in the conclusion.

2. Theory

Monte Carlo simulations couple two solvers: the criticality solver and the depletion solver. The criticality solver is used to solve the neutron flux and the depletion solver is used to solve the nuclide field. To solve these two coupled equations, it is approximated that the neutron flux is fixed in time, however this is not very practical since the neutron flux changes as the atomic concentration changes. Consequently, the equations cannot be used directly to determine the nuclide field at the end of the fuel cycle. In order to determine the atomic concentration and neutron flux of the system, the explicit Euler coupling scheme is used. The explicit Euler scheme starts by assuming a constant neutron flux when calculating the initial atomic concentration using the burnup equation. Then, the corresponding neutron flux is calculated using the criticality solver. As mentioned before, the neutron flux is assumed fixed, thus it is recommended to keep time steps short – when performing a simulation – since the neutron flux appear to be approximately constant leading to smaller errors.

Table 1 shows the algorithm for the explicit Euler method, where $\mathbb{M}$ is the transmutation matrix and Δt_i describes the time step dependence of the nuclide cross sections.

Email addresses: armansa@kth.se (Arman Salehi), febvre@kth.se (Romain Febvre)

[1]Both authors contributed to the paper equally.

Table 1. Algorithm of the explicit Euler method.

1:	**input:**	$\vec{N}_0$
2:	for	$i \leftarrow 0, 1, ... \, do$
3:		$\phi_i \leftarrow MC(\vec{N}_i)$
4:		$\vec{N}_{i+1} \leftarrow exp\left[\mathbb{M}(\phi_i)\Delta t_i\right]\vec{N}_i$
5:	end for	

The efficiency of the simulations ran are computed in terms of the figure of merit, FOM.

$$FOM = \frac{1}{\epsilon^2 C_{\Delta t}} \tag{1}$$

Where the $C_{\Delta t}$ is the computing cost of the Monte Carlo burnup simulation of the desired time period Δt and ϵ is the error of the Monte Carlo burn up simulation. For this study the error has been chosen as the concentration of Uranium-235 found in the burn up simulation after 365 days. The fraction of fuel left after a year of a simulation with optimum conditions is used as a reference and is used to find the error by finding its delta with simulations containing poorer statistics per step. In theory, ϵ could be any number, such as the error in effective multiplication factor (k_{eff}) or in the neutron flux. However, those values are specific to a single time step and cannot be used for the error of the whole simulation. In reactors with various burnable materials, the concentration of the higher actinide Plutonium is can be used, however in this study the only material present in the reactor at step 0 is Uranium, which fissions and does not favour the production of any material by a certain percentage, hence making the concentration of all its products random and unreliable as a source of error.

The reliance of the efficiency on the parameters can be explained by the functioning of each simulation. For example, a lower batch size means a faster computing time, but it will also cause an increase in the bias of the fission source.

Configuring the parameters to ensure the bias in the results are minimised whilst not enlarging the computing time by too much is important in minimising the sources of error such as the bias of the k-eigenvalue as well as non-convergence of the fission source.

3. Methodology

The test procedure described below allows to evaluate the optimised free parameters at each time step. The following procedure evaluates average computing cost and depletion cost at the beginning of the simulation via quick test criticality and depletion calculations. A reference simulation with small time steps is run to evaluate a burnup calculation with good statistics following a series of burnup simulations with larger (and varied) time steps. The material concentrations of each burnup simulation is evaluated. Finally, the error and figure of merit is then evaluated to find the optimal parameter.

It is desirable to evaluate each burnup simulation by a single figure of merit whereby the error evaluated should reflect the error in the depletion of the fuel material. As mentioned in Section 2, the error used to compute the figure of merit is the concentration of Uranium-235 after 365 days with different numbers of day steps. The value used is the standard deviation of said concentration from a reference simulation run with superior statistics than all the other simulation. The time step lengths and day steps are tabulated in Table 2. The computed error is expressed in Eq. (2).

$$\epsilon = \frac{|\,\vec{Z}_t - \vec{Z}_{ref}\,|}{|\,\vec{Z}_{ref}\,|} \tag{2}$$

Where Z_{ref} is the Uranium-235 concentration of the reference simulation after a year and Z_t is the Uranium-235 concentration after a year for a simulation with lesser statistics.

The procedure is implemented in the following fashion:

1. Run a quick Monte Carlo criticality simulation to evaluate the average computing cost of a single neutron history and depletion cost of the burnable material.
2. Run a reference Monte Carlo criticality simulation with a small time step (e.g. 1 day step for 365 days) in order to obtain good statistics.
3. Run a series of burnup simulations for various time steps (see Table 2).
4. Obtain the material concentration from the depletion simulation of each burnup simulation and evaluate the depletion cost.
5. Set the depletion and initialisation cost fraction to a user-specified value.
6. Evaluate the error from the material atomic concentration given by Eq. (2).
7. Evaluate FOM and plot with respect to depletion to the total cost of the burnup simulations.

Table 2. Simulation set specification of different time step lengths.

Time step length	Number of day steps
1 day (reference)	365
7 days	52
14 days	26
26 days	14
31 days	12
46 days	8
61 days	6
73 days	5
91 days	4

Table 3. Constant specification common to all simulations.

Simulation set	Total number of neutrons in each set
Set #1	10^5
Set #2	10^7

Table 4. Constant specification common to all simulations.

Variable	Value
Total time period	365 days
Total number of neutrons per simulation	10^7
Number of active cycles	1000
Equilibrium xenon	Set on

3.1. Results

Test simulations were carried out in order to determine the figure of merit, however the total cost and depletion cost have to known. These values depend on different factors such as the model geometry complexity, the number of burnable material and nuclides in the various materials, the speed and number of CPUs as well as the efficiency of the computing scheme. Nevertheless, various values of the depletion cost and overall cost fraction was chosen in order to map how this ratio affects figure of merit of each simulation.

Two sets of simulations were carried out with different total number of neutrons as shown in Table 3. However, the individual set simulations sampled the same total number of neutrons and time period in each of the varied time step lengths (see Table 4). No inactive cycles have been set in any of the burnup simulations.

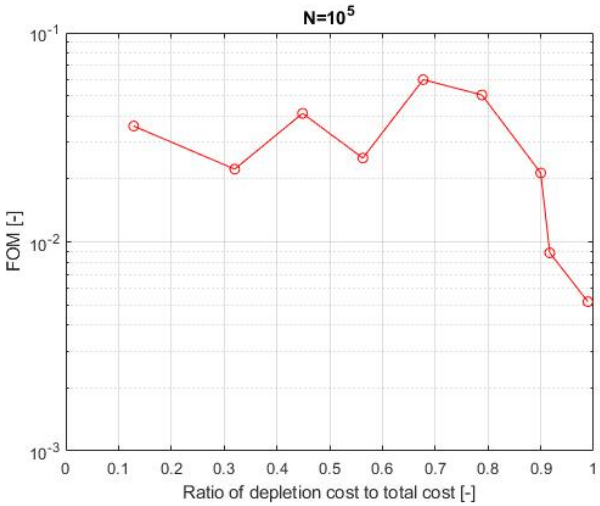

Figure 1. Figure of merit simulated for 10^5 neutrons.

The simulation sets differ in total number of sampled neutrons. The results are presented below in Fig. 1 and Fig. 2. The figure of merit is plotted against the ratio of depletion time to overall running time. Each point gives the figure of merit of a different burnup simulation with a specific time step. Simulations with small values of cost fraction ratio have relatively large time steps. As the cost fraction ratio increases, the time step decreases.

Simulations in Set #1, shown in Fig. 1, achieved best efficiency between the interval (0.6, 0.8), whereas simulations in Set #2, shown in Fig. 2, achieved best efficiency between the interval (0.3, 0.5),

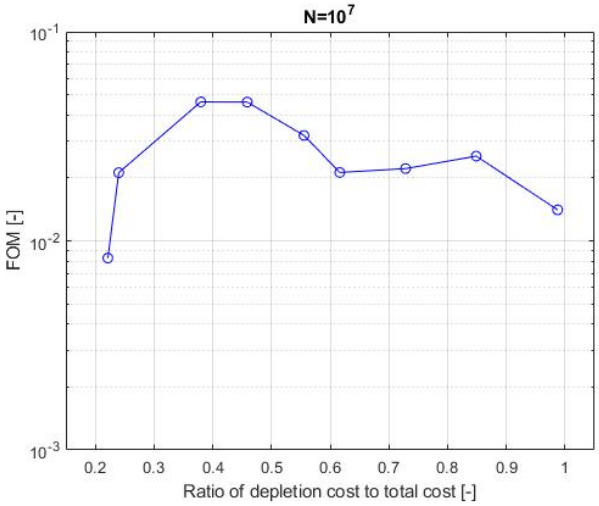

Figure 2. Figure of merit simulated for 10^7 neutrons.

4. Discussion and conclusion

The results obtained from the test numerical simulations demonstrates that the depletion and overall cost fraction ratio can be a very useful parameter to determine the optimisation of free parameters of Monte Carlo burnup simulations. While some free parameters can be optimised automatically, as was shown in J. Dufek and I. Mickus (2020), the user still needs to set certain parameters such as the number of neutrons simulated per criticality cycle. This was done in both set simulations. Set #1 ($N = 10^5$) showed the best efficiency between the interval (0.6, 0.7) and Set #2 ($N = 10^7$) between the interval (0.3, 0.4).

The explicit Euler coupling scheme allow the user to set the depletion run times. The scheme calculates the neutron flux at the beginning of a time step and depletes materials with the flux over the whole time step. The process repeats until the end of the time period is reached. It would be reasonable to set a large value of depletion run times in order to obtain the neutron flux, if required, as the neutron flux will be combined over a large number of Monte Carlo criticality runs at each time step. However, if the neutron flux is not required to be among the results at each step, it is recommended that the value of the depletion time run be kept small as it keeps the time steps short along with the spectral changes over the time steps.

The accuracy of the results can be improved if the computing time was set to a large value. Thereby combining the computing power of several hundred or thousands of processors, results with good accuracy can be obtained. For the set simulations carried out in this study, a limit of 4 servers enforced.

More simulations must be run to test the reproducibility of the results above as well as adding more computing power to achieve better accurate results. Furthermore, the inactive cycles were not treated in this study which can be addressed in future studies.

References

Dufek, J. and Mickus, I., 2020. Optimal time step length and statistics in Monte Carlo burnup simulations. Annals of Nuclear Energy, 139, 4–7.

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