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OpenMC(TD): Current status and next development stages

Jaime Romero-Barrientos[1,2,*], *Francisco* Molina[1,2,3], *Marcelo* Zambra[1,4], and *Franco* López-Usquiano[1,3]

[1]Centro de Investigación en Física Nuclear y Espectroscopía de Neutrones CEFNEN, Comisión Chilena de Energía Nuclear, Nueva Bilbao 12501, Las Condes, Santiago, Chile.
[2]Millennium Institute for Subatomic physics at high energy frontier - SAPHIR, Fernández Concha 700, Las Condes, Santiago, Chile.
[3]Departamento de Ciencias Físicas, Universidad Andres Bello, Sazié 2212, 837-0136, Santiago, Chile.
[4]Universidad Diego Portales, Manuel Rodríguez Sur 415, Santiago, Chile.

Abstract. This work presents the current state and the next stages in the development of the modified code OpenMC(TD), a modified version of the Monte Carlo code OpenMC which includes the time dependence related to the emission of β-delayed neutrons, but instead of simulating these neutrons using the traditional 6-group structure, features an implementation where individual precursors decay. This code is in active development, but already shows promising results. The upcoming development stages for OpenMC(TD) have two complimentary aspects, one related to the Monte Carlo code and another related to experimental measurements at a research nuclear reactor. Regarding the code, it is planned to implement the branchless collision variance reduction technique, while to validate the simulations, transient experiments will be performed at the RECH-1 research nuclear reactor.

1 Introduction

Traditionally, Monte Carlo codes are used in reactor physics to study stationary problems, but in recent years there have been efforts to develop pure Monte Carlo codes that can study transient or kinetic phenomena. Serpent [1], two extensions for TRIPOLI-4 [2], by Sjenitzer and Hoogenboom [3] and by Faucher [4], the GUARDYAN code [5], the G4-STORK [6] class for GEANT4 [7] and the transient module by Milonakis [8], are some of the codes recently developed that include the time dependence related to the emission of β-delayed neutrons. One trait that all of these Monte Carlo codes have in common is that they use the traditional group structure proposed originally by Keepin, gathering all β-delayed precursors in 6 families. Although this grouping is routinely used, nowadays, and given the rise in computing power and the availability of nuclear data, it is possible to simulate the β-delayed emission from individual precursors, so that the effect of individual precursor data in reactor calculations can be explored. These two features, the inclusion of time dependence and the use of individual precursors, characterize the modified code OpenMC(TD) [9, 10]. This work presents, on one hand, a summary of the current development stage of the modified Monte Carlo code OpenMC(TD), and in the other hand, the next development phases, which are

*e-mail: jaime.romero@cchen.cl

related to the implementation of the variance reduction technique called branchless collision and the transient experiments planned in the research reactor RECH-1 that will serve as experimental benchmarks to validate the simulation results.

2 About OpenMC(TD)

In deterministic and Monte Carlo neutron transport codes, the emission of β-delayed neutrons is implemented using a group structure, where β-delayed neutron precursors are grouped in 6 (or 8) groups. As an example, from the fission of ^{235}U there exists about 270 precursors, but all of these β-delayed precursors are gathered in 6 groups. Each one of these groups consists of a variety of isotopes, and is characterized by: i) a decay constant, ii) a relative yield, and iii) an energy spectrum [11]. Although this aggregation is routinely employed in nuclear reactor codes, this grouping limits the opportunity of studying the impact that individual nuclear data from precursors can have on Monte Carlo simulations of nuclear reactors. Moreover, the emission of β-delayed neutrons happens between 10^{-3} s to 10^{2} s after the decay of the precursor. Therefore, the time dependence associated with β-delayed neutron emission has to be included in a Monte Carlo simulation. This is challenging, because it requires simulating events that are order of magnitude different, situation that results in large variances. More specifically, the emission of prompt neutrons occurs almost instantaneously (10^{-14} s after fission), while delayed neutrons are emitted in times several order of magnitude larger. Taking this into account, modifications were made to the OpenMC code to include: i) the time dependence associated with the β-delayed emission, and ii) the decay of individual precursors, instead of using the traditional group structure. The modified code was named Time-Dependent OpenMC or OpenMC(TD) Monte Carlo code [9, 10] and it was intended as a first step towards the development of a tool to explore the effect of individual precursor data in transient simulations. Even though these modifications are described in further detail in a previous publication [10], a brief summary of its main aspects is presented:

1. ***Time dependence in Monte Carlo:*** Since time is not included in an explicit manner in a Monte Carlo simulation, the first step was to add a time label to account for the time evolution of the neutrons. To score the time evolution of quantities in the simulation (e.g. neutron flux as a function of time), a *time filter* was developed to add the capability of monitoring the time evolution of the tallies present in the code. Lastly, the total simulation time was divided in discrete time intervals. The reason behind this, is that the variance reduction and population control methods implemented require a *time grid* to be applied. Also, in transient simulation changes in the reactivity or geometry can occur, and these changes can be established at the end of a time interval.

2. ***β-delayed emission from individual precursors:*** At the time of this writing, apart from OpenMC(TD), no published MC codes with β-delayed emission from individual precursors could be found. What MC codes do, is that, if a delayed fission is sampled, then it is chosen which delayed group will be sampled. After selecting the corresponding group, the delayed time associated with the delayed emission is sampled. Regarding the delayed neutron energy, it is sampled from the delayed neutron energy group spectrum, and then the delayed neutron is inserted in the simulation. In OpenMC(TD), a precursor is created if a delayed neutron is sampled. After that, the individual precursor that will decay is chosen. To achieve this, the precursor *importance* or relative abundance of the i-th individual precursor, I_i, is defined as [12]

$$I_i = \frac{CY_i \, P_{n,i}}{\nu_d}, \tag{1}$$

with CY_i the cumulative fission yield, $P_{n,i}$ the precursor delayed neutron emission probability, and ν_d the average delayed neutron yield. After having selected the corresponding individual precursor, the delayed time associated with the emission is sampled. Finally, the delayed neutron energy is the average energy from sampled from the corresponding precursor delayed energy spectrum.

3. ***Time delay of β-delayed neutron emission:*** To address the time delay of delayed neutron emission and obtain meaningful results, the *forced decay* [3] and *combing* [13] method were implemented in OpenMC(TD). In the *forced decay* method, the precursor decay probability is changed, forcing the decay of all the precursors in each interval, thus increasing the number of delayed neutrons. Since the sampling of delayed neutrons is biased, Monte Carlo fair game must be preserved by changing the statistical weight of the delayed neutrons. Given that in the *forced decay* method precursors are always kept in the simulation after they decay into delayed neutrons, their number increases as the simulation advances, so the precursor population needs to be controlled. This was accomplished by using the *combing method*, which is a population control method which preserves the total statistical weight, while keeping a fixed number of particles, where all the statistical weights are set to be the average weight.

As part of the development process, OpenMC(TD) was tested in a series of successively complex systems. A detailed description of these tests and its results can be found in [10]. These tests were successful, although the wall-clock times were high, so the next development stages are focused on solving this issue, by implementing further variance reduction methods.

3 Next developing steps

3.1 OpenMC(TD) development

The features of OpenMC(TD) presented in Sec. 2 were implemented in version 0.10, which was written in FORTRAN. So, the first steps towards continuing the development of OpenMC(TD) are to translate the code to its current language in C++, work that is currently underway. After the translation to C++ is done, the next development steps are to implement variance reduction schemes in order to optimize the calculation speed, testing of the aforementioned variance reduction implementations in simple systems and running the simulation of a full research reactor core in a supercomputer. A brief description of each one of these steps is presented:

3.1.1 Branchless collisions

Although OpenMC(TD) currently features two implemented variance reduction methods, *forced decay* and *combing*, in order to further reduce the variance and speed up the results, an additional variance reduction scheme will be implemented: the branchless collision method [14, 15]. The idea behind this method is that when a scattering or fission reaction occurs, only one particle is emitted. In this method the statistical weight w' of the particle that emerges from the interaction is independent of the reaction and is given by

$$w' = w\frac{\nu_f\Sigma_f + \Sigma_s}{\Sigma_t}, \tag{2}$$

where w is the particle original weight, ν_f is the average number of neutrons produced per fission, and Σ_f, Σ_s and Σ_t are the macroscopic fission, scattering and total cross sections,

respectively. Since the statistical weight of the particle is the same regardless of the reaction, collision probabilities changes. Indeed, we have that the modified scattering probability is

$$P_s = \frac{\Sigma_s}{\nu_f \Sigma_f + \Sigma_s}, \tag{3}$$

while the modified fission probability is

$$P_f = \frac{\nu_f \Sigma_f}{\nu_f \Sigma_f + \Sigma_s}. \tag{4}$$

3.1.2 Testing

After the implementation of the branchless method in OpenMC(TD), the next step in the development plan is to test the code by running transient simulations in a variety of simple systems. The objective of this stage is twofold: first, to quantify the effect of the different variance reduction schemes implemented in the code by measuring the wall-clock time and the figure of merit; and second, to advance towards a scalability study, which is necessary to apply for computing time on the Guacolda-Leftraru supercomputer, which belongs to The National Laboratory for High Performance Computing [16] (NLHPC), where a transient simulation of a full reactor core will be performed. If possible, results at this stage could be compared to results obtained using other Monte Carlo codes with kinetic capabilities.

3.1.3 Simulations on supercomputer

The last stage in the development plan for OpenMC(TD) is to run a transient simulation of a full research reactor core. For this case, and given that this project aims to also propose transient benchmark experiments (see Sec.3.2), the core to be simulated corresponds to the research reactor RECH-1 [17].

3.2 RECH-1 research reactor benchmark experiments

As mentioned in Sec. 1, along with the development of the code, this project entails experiments in the Chilean nuclear research reactor RECH-1. The objective of these experimental measurements is to verify the time dependence of the neutron flux in simple experiments, such as the insertion or removal of reactivity in an irradiation position. To perform these measurements at a nuclear reactor there are some requirements needed to be considered: access to the nuclear reactor, availability of the reactor operators, the presence of a radiological protection officer according to current regulation and exclusive allocated time. The proposed measurements needed to benchmark the results from transient Monte Carlo simulations are the time change in reactor flux due to the insertion or removal of reactivity into and from the core, respectively. To achieve this change in reactivity it is proposed: i) to insert or withdraw the control plates, or ii) by insert a small absorber using the available rabbit system (feasibility of this experience needs to be confirmed) or through the dry tube irradiation facility. In any case, the idea is to experimentally account for changes in neutron flux due to the insertion or removal of reactivity that can be simulated using OpenMC(TD). Given that the estimated prompt generation time of a nuclear research reactor is of about 60 μs, then the temporal resolution needed to describe the decay or rise of the neutron flux is of about 1 μs, resolution achievable with the available detection and acquisition systems. Two detector systems are proposed to measure the time dependence of the neutron flux. The first one is an in-core Self

Powered Neutron Detector (SPND), coupled with a picoammeter with time resolution of the order of μs, which will be located inside the RECH-1 core. The second one is an available ex-core He-3 neutron detector, which can be located, for example, in a neutron beam line. In addition to these detectors, a reactimeter is available to monitor the time change of the neutron population. It is important to mention that the burn up state of the core's nuclear fuel needs to be considered. To take this into account, calculations using CITATION [18] and WIMS [19] codes can be performed if needed to calculate the new isotopic composition of the nuclear fuel, which will be used during the construction of the geometry of the simulation.

4 Conclusions

This work presented a summary of the current status in the development of the modified code OpenMC(TD), which is a modified version of OpenMC which includes the time dependence related to the β-delayed neutron emission from individual precursors, instead of using the traditional precursor group structure. In the first stage of the development, time was included explicitly in the simulation, the total simulation time was divided into discrete time intervals, and a *time filter* was developed to monitor the time evolution of quantities of interest (e.g., neutron flux). After the inclusion of time, individual precursors were included in the code. To achieve this, an *importance* or relative abundance was defined for each precursor, using its cumulative fission yield, its delayed neutron emission probability and the average delayed neutron yield. Finally, β-delayed emission from individual precursors was addressed by using the variance reduction technique known as *forced decay*, where all of the precursors are forced to decay at the beginning of each time interval. Since in the *forced decay* method the precursors are kept in the simulation after they decay, population control has to be enforced. This was done using the *combing method*, which preserves the total statistical weight while keeping a fixed number of particles. These implementations were tested successfully in various systems. The next steps in OpenMC(TD) development are to implement the branchless collision method, so variance can be further reduced. Then it is planned to test the new implementations on simple systems, and after successful testing, a transient simulation of the RECH-1 nuclear reactor core will be run in a supercomputer. In parallel, transient experiments will be performed at the RECH-1 reactor, to benchmark the transient simulation. The idea is to propose a set of transient benchmarks for the verification of future Monte Carlo transient codes. It is expected that OpenMC(TD) can serve as a tool to prompt new measurements of experimental data on β-delayed neutron emission.

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