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Particle clustering in Monte Carlo criticality simulations

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ABSTRACT

Strong space and cycle correlations affecting the neutron flux have been recently reported to occur in Monte Carlo criticality simulations of pressurized water reactors pin-cells with reflective boundary conditions: when the system size is large, neutrons are observed to gather together and form ‘clusters’ that wander around in space over many cycles. In most cases, the outcome of such clustering is that simulations display wild fluctuations, largely exceeding those expected around the equilibrium distribution. In this paper, we analyze the reasons behind the emergence of these phenomena: we show that the key mechanism is due to the asymmetry between neutron disappearance being uniformly distributed along the pin-cell, and neutron generation being localized at fission sites (i.e., only next to a parent particle). An explanation is provided by resorting to a simplified Brownian transport model coupled with a Galton–Watson birth and death process, which is sufficient to retain the essential features observed in realistic Monte Carlo simulations. An empirical space correlation function is proposed as a diagnostic tool for detecting clustering in criticality simulations.

1. Introduction

Monte Carlo particle transport methods are widely adopted as the reference tool for simulating complex nuclear systems as accurately as possible. Accuracy is defined in terms of introducing a limited number (possibly none) of approximations concerning the system geometry, energy and angular distributions of the transported particles, and so on (Lux and Koblinger, 1991; Brown, 2005).

In particular, Monte Carlo methods are extensively used in the domain of reactor physics. In this context, the workhorse of Monte Carlo methods for criticality calculations is the stochastic version of the so-called power iteration algorithm (Duderstadt and Hamilton, 1976; Bell and Glasstone, 1970; Lux and Koblinger, 1991; Rief and Kschwendt, 1967; Brown, 2005), whose basic idea is to follow neutrons along generations (cycles), starting with a birth from a fission event and terminating when the neutron is lost by either leakage from the outer boundaries or absorption (including sterile captures and fissions). In between, neutrons are tracked along their random trajectories through the traversed media. Such ‘cycles’ are started from an arbitrary source and are iterated until the neutron population ultimately converges to a stable shape in both space and energy at some late generation. Once convergence has been attained, recording the appropriate estimators and taking the averages over all random realisations allows computing flux profiles, reaction rates, and other physical quantities of interest (Lux and Koblinger, 1991).

Such Monte Carlo scores correspond by definition to averages over a given element of phase space (typically, spatial volumes and energy intervals). Fluctuations around average values appear because of Monte Carlo simulations being intrinsically based on the transport of a finite number of particles: by increasing the number of simulated histories, it is well known that the fluctuations affecting the computed scores are progressively reduced (Lux and Koblinger, 1991; Brown, 2005). Another source of noise specific to Monte Carlo criticality calculations is related to fission events, because of two concurrent phenomena: (i) fissions induce splitting of the trajectories, which increases the dispersion of the population number within a given volume; and (ii) the birth of a neutron occurring at a fission site induces correlations between particle positions (Lux and Koblinger, 1991; Sjenitzer and Hoogenboom, 2011). Overall, the convergence of Monte Carlo scores to their respective average values will demand a larger number of generations, and in some cases it is even possible that convergence is never achieved (especially when the number of simulated particles is relatively small) (Brown, 2005). Understanding and quantifying these phenomena is a task of utmost importance so as to improve the reliability of Monte Carlo criticality calculations.

The goal of this paper is to address the mechanisms that are responsible for the above-mentioned fluctuations: we will show that the key reason behind these fluctuations is indeed a source convergence problem mainly due to undersampling. Since the

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extent of such fluctuations over spatial volumes and over cycles is strongly problem-dependent, in Section 2 we begin by considering a specific example, namely, the simulation of a pressurized water reactor (PWR) pin-cell configuration. Then, in Section 3 we analyse a simple stochastic particle transport model that allows singling out the key mechanisms underlying space and cycle fluctuations. On the basis of these considerations, in Section 4 we propose a Monte Carlo estimator well suited for the diagnostic of criticality simulations. Conclusions and perspectives are finally presented Section 5.

2. A representative example: a PWR pincell

In order to illustrate the issues mentioned above, in this section we consider a simple test case, namely a criticality Monte Carlo simulation of a PWR pin-cell. Monte Carlo simulations are performed by resorting to the Tripoli-4® multi-purpose continuous-energy code developed at CEA/Saclay (Brun et al., 2011; Tripoli-4 Project Team, 2008). The pin-cell system, as customary, is composed of a single UO_2 fuel rod (at 3.25% enrichment) of radius 0.407 cm. The fuel rod is enclosed in a Zircaloy cladding of outer radius 0.477 cm, and a water moderator surrounds the cladding. All materials are kept at 300 K. For a two-dimensional cut view of this configuration, see Fig. 1. For Monte Carlo simulations, reflective boundary conditions are applied on the pin-cell, so that the expected equilibrium distribution for the flux is axially flat in space. As for the number of particles, we have run each simulation for 10^3 cycles with 10^4 neutrons per cycle, with a spatially uniform initial guess source.

Convergence of the criticality cycles (the power iteration algorithm) is monitored by measuring the effective multiplication factor (*keff*) at each cycle. Monte Carlo scores are recorded after convergence on *keff* has been attained. For the simple case considered here, convergence of *keff* is typically achieved within very few cycles. At the end of each cycle after convergence, the neutron flux is recorded over a regular spatial grid composed of 40 bins along the axial direction. Three sets of simulations are run, by varying the axial length of the pin-cell (all the other physical parameters being kept constant).

In the first simulation, a pin-cell length $L = 10$ cm is chosen, and the corresponding neutron flux (in arbitrary units) is shown in Fig. 2 (left). The flux is plotted as a function of the spatial binning at each cycle. Fig. 2 (left) clearly shows that the flux stays uniform in space all along the cycles, and that fluctuations around the average value are fairly small.

In the second simulation, the pin-cell length is increased to $L = 100$ cm. In this case, Fig. 2 (center) shows that the neutron flux suffers from much stronger fluctuations in space, which moreover evolve as a function of the cycles. These fluctuations are not localized and their size clearly extends to the whole domain length.

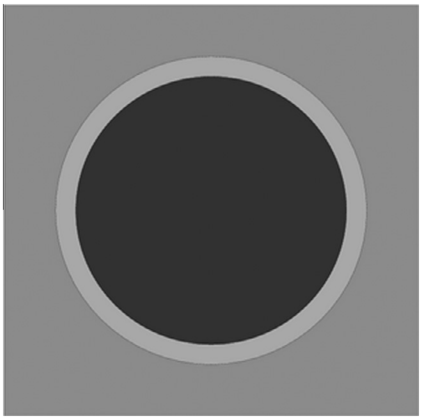

Fig. 1. A transversal cut of the PWR pin-cell. The moderator has a size $R = 1.26$ cm.

This behavior is further enhanced when taking $L = 400$ cm, as shown in Fig. 2 (right). In this case, fluctuations become even more important, and completely override the average flux value, so that (loosely speaking) it is no more possible to properly define an equilibrium flux distribution. In particular, the flux distribution has not converged in space, despite the multiplication factor having reached a stationary value. Fig. 2 (right) reveals a very interesting feature: the overall effect of these fluctuations is that neutrons gather into *clusters*, and empty 'holes' appear between them. While the total neutron population is preserved, the spatial distribution is strongly heterogeneous and randomly evolves along the cycles: in other words, the neutron clusters seem to wander around indefinitely.

This simple example shows that for large systems with a mild number of simulated particles monitoring the convergence of the effective multiplication factor might be misleading, since the spatial distribution of the neutron flux might not even achieve convergence. This clustering effect is amplified by increasing the system dimensions, when keeping fixed the number of simulated particles.

3. Space and cycle fluctuations analysis

The analysis of neutron flux fluctuations at a given spatial site as a function of cycles has been discussed at length in literature (see for instance (Ueki, 2012; Brown, 2009)). The impact of such fluctuations has been widely recognized, in that they affect the convergence of Monte Carlo scores by introducing cycle-to-cycle correlations, which in turn make the applicability of Central Limit Theorem questionable. Such correlations along cycles have been often studied within the mathematical framework provided by the eigenvalues analysis of the Boltzmann critical equation (Brown, 2005). Further work on correlations has concerned techniques aimed at improving the standard deviation estimates of Monte Carlo scores (Gelbard and Prael, 1990; Jacquet et al., 2000; Ueki et al., 2003; Ueki et al., 2004; Dumonteil and Malvagi, 2012). In order to detect fluctuations along cycles, effective diagnostic tools have been developed for Monte Carlo simulations, among which a prominent role is played by the so-called entropy (Ueki and Brown, 2003; Dumonteil et al., 2006; L'Abbate et al., 2007).

However, an analysis based on cycle fluctuations alone (by averaging out or simply neglecting the spatial behavior) fails in interpreting the features that we have singled out in the pin-cell example discussed above. For instance, the cycle-to-cycle entropy estimator would be inefficient in detecting neutron spatial clustering (Dumonteil and Courau, 2010). The coupling between space and cycle fluctuations has been the subject of some recent investigations (Dumonteil and Malvagi, 2012). A tentative explanation has been provided in terms of the excitation of higher harmonics of the neutron flux spatial distribution by the statistical noise. Two main features have been singled out: (a) fluctuations are more relevant in systems with high dominance ratio; and (b) fluctuations decrease by increasing the number of simulated neutrons per unit volume. This analysis has nonetheless shown that reliable tools for quantifying the impact of space and cycle fluctuations are still missing.

A complete description of cycle and space fluctuations of the Monte Carlo particle population would demand in principle the sophisticated tools provided by statistical mechanics and the theory of Monte Carlo games. In this respect, one would need to develop formulas for the average, the variance, and the correlation function of the number of particles at a given site and cycle by using the framework of branching processes and neutron noise