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Original Article

Clustering and traveling waves in the Monte Carlo criticality simulation of decoupled and confined media

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ABSTRACT

The Monte Carlo criticality simulation of decoupled systems, as for instance in large reactor cores, has been a challenging issue for a long time. In particular, due to limited computer time resources, the number of neutrons simulated per generation is still many order of magnitudes below realistic statistics, even during the start-up phases of reactors. This limited number of neutrons triggers a strong clustering effect of the neutron population that affects Monte Carlo tallies. Below a certain threshold, not only is the variance affected but also the estimation of the eigenvectors. In this paper we will build a time-dependent diffusion equation that takes into account both spatial correlations and population control (fixed number of neutrons along generations). We will show that its solution obeys a traveling wave dynamic, and we will discuss the mechanism that explains this biasing of local tallies whenever leakage boundary conditions are applied to the system.

1. Introduction

Monte Carlo neutron transport codes [1,2] are often used as a reference tool by the nuclear industry, as the approximations on which they rely to solve the Boltzmann equation in fissile media (the so-called critical Boltzmann equation [3]) are extremely sparse. Their growing use in the past few decades is strongly correlated to the increase of computer resources and now ranges from nuclear fuel cycle studies to criticality safety assessment and reactor physics simulations. However, in this last application, and especially in the case of large reactor cores or loosely coupled systems [4,5], a strong undersampling effect biases the estimates of the variance of flux-based quantities [6—10]. Worse, in a work inspired by recent developments in population ecology [11—14], Dumonteil, Mazzolo and Zoia have shown that non-Poisson spatial fluctuations were caused by a neutron clustering phenomenon [15—18]: even for intermediate or high numbers of simulated neutrons, those fluctuations can make it hard to estimate flux-based standard deviations. The very first description of this mechanism typical of birth—death processes dates back to the 1980s, when Cox and Griffeath [19] showed that the spatial correlations affecting some branching processes evolving in infinite media in dimension 1 or 2 were diverging in amplitudes, while in dimension 3 those spatial correlations would saturate. Later on, while being translated from the field of probabilities to the fields of population ecology (describing spatial patterns appearing in water column plankton [11] or describing bacterial growth in Petri dishes [13,14]), neutron transport [15,16], and statistical mechanics [17,18], this process was referred to as clustering or Brownian bugs, whether it be for finite or infinite media in any dimension and with different kinds of boundary conditions. In the present paper, we will show that space-dependent biases observed while simulating the neutron transport in decoupled systems find their origin in these spatial correlations, when leakage boundary conditions are employed. Section 2 will discuss the phenomenology of these biases on a commercial reactor benchmark, and on a simplified model grasping its main characteristics [the mass-preserved one-dimensional (1D) binary branching Brownian motion on a segment with Dirichlet boundary conditions]. In Section 3 we will build a functional equation modeling the simplified case, based on a generalized Fisher equation with time-dependent coefficients that accounts for population control and which incorporates spatial correlations. In Section 4 we will rely on an asymptotic analysis to establish a deep connection between traveling waves proper to quadratic terms in the neutronic field equation and clustering. In particular, we will show that the neutron clusters trigger a traveling

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wave dynamic on the flux causing the bias on local tallies. Some numerical solutions of this equation retrieved under simplifying hypotheses will be compared to the numerical findings of the first section. Conclusions will be drawn in the final section.

2. Biases associated to the Monte Carlo simulation of large reactor cores

2.1. Commercial reactor critical benchmark

The Expert Group on Advanced Monte Carlo Techniques belongs to the Working Party on Nuclear Criticality Safety of the OECD Nuclear Energy Agency. Its aim is, amongst others, to guide Monte Carlo criticality practitioners through finding their ways in defining the most appropriate simulation parameters, so as to minimize biases in the Monte Carlo estimate of different local quantities or in the estimate of their variances. This group, as well as recent work, has pointed out strong bias in both the estimate of the flux and its variance, which depends on the spatial position of the tally volume [20,21]. This bias is prone to develop in particular for loosely coupled systems. Thus, a benchmark named R1 is currently under study, which proposes to tally the flux in different radial zones of a critical commercial reactor [22]. This reactor has been simulated with the MORET 5.B.2 Monte Carlo code [23], exploiting a quarter symmetry. Axially averaged fluxes are presented on the left part of Fig. 1 and the associated "apparent" 1-σ error bars are provided by the left plot of Fig. 2 (these error bars are calculated by the Monte Carlo code using the central limit theorem). As expected, the highest uncertainties are located in low flux regions, where neutrons leak out of the core. Surprisingly enough, though, the "true" error bars given by the right plot of Fig. 2 exhibit spatial patterns: these errors seem to be big near the leaking boundaries of the reactor core but are also close to the reflecting boundaries and at the center of the core. Such nontrivial spatial patterns are even more striking on the right plot of Fig. 1, where the undersampling bias is estimated and is shown to be bigger at the center of the core, and close to the leaking boundaries. In particular, the flux is overestimated near the leaking edges and is underestimated at the center. Also, the amplitude of this bias, be it positive or negative, seems to be inversely proportional to the number of neutrons per generation, as revealed by Fig. 3 In the following parts of this paper, we will try to model this very last phenomenon, also reported by many authors and papers.

2.2. Mass preserving branching Brownian motion on a 1D confined medium with Dirichlet boundary conditions

In order to explain these observations, different capabilities of the MORET 5.B.2 Monte Carlo code were successively disabled (simplified geometry, one group cross-sections, etc.) to grasp the phenomenology discussed in the present paper with the simplest model. In this respect it appeared that a mass-preserving binary branching Brownian motion [19,24,25] on a segment (of half length L arbitrarily set to 20) with Dirichlet (leakage) boundary conditions allowed to observe precisely an underestimation of the flux in the central region while reproducing an overestimation of the flux close to the boundaries. It is worth noting that such a modeling is more suited to Monte Carlo dynamic simulations (which make use of an algorithmic loop over time steps instead of a loop over neutron generations): for that reason a methodology to model generation-based simulations directly, instead of time-dependent problems, was proposed in a very recent work [26]. However, for the particular phenomenon described in this paper no significant differences were observed between criticality and dynamic simulations: continuous time processes will be used as a means to draw conclusions that apply to both processes. The mass-preserving mechanism used in the simulations is fully described [27,28,18]. It is based on a combination between splitting and Russian roulette techniques: each time a particle is captured by a physics process, another is picked randomly and split, while each time a fission occurs, a randomly picked particle is Russian rouletted. The diffusion coefficient D was set to 1, while the binary process was such that the capture cross-section γ was equal to the two-daughter particles fission cross-section β, and both were set to 0.1. Typical realizations of such a process are provided in Fig. 4. As expected, the top plot of this figure highlights a strong particle clustering mechanism [16], and reveals that, after a short time, only one cluster remains [17]. Interestingly enough, though, looking at this process on a large time window (bottom plot), a qualitative view of the problem under consideration emerges: when only one cluster of particles strikes one of the boundaries while wandering around, the constraint on the overall mass N of our mass-preserving process refrains the particle cluster from leaking out of the system, the splitting rate increases dramatically until the cluster is "reflected" to the other side of the system. Therefore the Dirichlet boundary conditions cannot be properly taken into account. When the system is not prone to trigger a clustering effect (i.e., for coupled

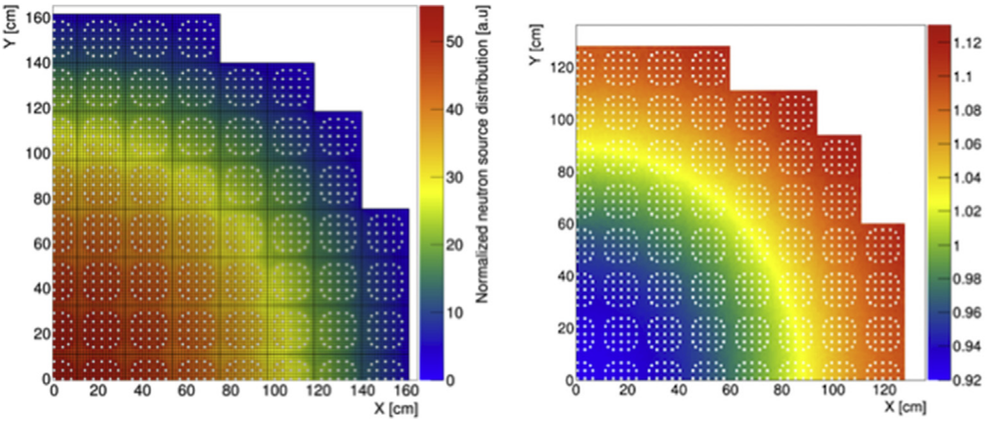

Fig. 1. MORET 5.B.2 simulation of the R1 OECD/NEA benchmark: axially averaged fluxes with 10^4 active cycles of 10^4 neutrons (left plot). Ratio of the axially averaged fluxes between a simulation with 10^6 active cycles of 10^2 neutrons and a simulation with 10^2 active cycles of 10^6 neutrons (right plot).