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Monte Carlo power iteration: Entropy and spatial correlations

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ABSTRACT

The behavior of Monte Carlo criticality simulations is often assessed by examining the convergence of the so-called entropy function. In this work, we shall show that the entropy function may lead to a misleading interpretation, and that potential issues occur when spatial correlations induced by fission events are important. We will support our analysis by examining the higher-order moments of the entropy function and the center of mass of the neutron population. Within the framework of a simplified model based on branching processes, we will relate the behavior of the spatial fluctuations of the fission chains to the key parameters of the simulated system, namely, the number of particles per generation, the reactor size and the migration area. Numerical simulations of a fuel rod and of a whole core suggest that the obtained results are quite general and hold true also for real-world applications.

1. Introduction

Monte-Carlo simulation is often used in criticality calculations to assess the asymptotic distribution of the neutron population within a system, which corresponds to the fundamental eigenmode of the Boltzmann critical equation (Lux and Koblinger, 1991). The most widely used and simplest numerical method allowing the neutron population to converge to the fundamental eigenmode is the power iteration (Lux and Koblinger, 1991; Rief and Kschwendt, 1967; Brown, 2005): in Monte Carlo methods, an initial arbitrary source particle distribution is transported until all neutrons have been either absorbed or leaked (forming a so-called generation). The secondary neutrons coming from the fission events within a generation g are banked and provide the source for the following generation $g+1$. The algorithm is then iterated over many generations, until the fission sources for a sufficiently large g statistically attain a spatial and energetic equilibrium, as ensured by the power iteration method. The effects of higher eigenmodes on the neutron population are expected to fade away, and eventually the neutron population will be distributed according to the fundamental eigenmode. The ratio between the population size at generation $g+1$ and the population size at generation g converges to the fundamental eigenvalue k_{eff} for large g (Lux and Koblinger, 1991).

In this context, two key issues are known to affect the neutron population during power iteration and have therefore attracted intensive research efforts: fission source convergence and correlations.

Concerning the former, a slow exploration of the viable phase space by the population implies a poor source convergence. In particular, it has been shown that the convergence of k_{eff} might be faster than that of the associated fundamental eigenmode, which is expected on physical grounds, the former being an integral property of the system and the latter being a local property (Lux and Koblinger, 1991). The rate of convergence depends on the separation between the first and the second eigenvalue of the Boltzmann equation, the so-called dominance ratio: the closer to one the dominance ratio becomes, the poorer the convergence (Lux and Koblinger, 1991; Ueki et al., 2004; Dumonteil and Malvagi, 2012). If Monte-Carlo tallies are scored before attaining equilibrium, biases on the estimation of the variance may appear, and monitoring the convergence of k_{eff} might be insufficient so as to determine the convergence of the whole population (Ueki and Brown, 2003; Dumonteil et al., 2006; L'Abbate et al., 2007; Ueki, 2005).

Several tools have been proposed to assess the spatial convergence of fission sources, among which, one of the most popular, is the entropy of the fission sources (Ueki et al., 2003; Ueki, 2012; Ueki and Brown, 2003; Ueki, 2005). The idea behind the entropy function is to superimpose a regular Cartesian mesh to the viable space and to record the number of fission sites for each

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cell of the mesh, at each generation. This allows computing the so-called Shannon entropy $\mathcal{S}$ (Li and Vitanyi, 1997), which is defined as

$$\mathcal{S}(g) = -\sum_{i,j,k} p_{i,j,k}(g)\log_2[p_{i,j,k}(g)], \quad (1)$$

where $p_{i,j,k}(g)$ is the (statistically weighted) number of fission source particles in the cell of index i,j,k at generation g divided by the total number of source particles in all cells at generation g. The entropy function is expected to provide a measure of the phase space exploration as a function of the number of generations (Li and Vitanyi, 1997; Cover and Thomas, 1991): when the neutron distribution attains its stationary shape, the entropy $\mathcal{S}$ converges. A prominent advantage of the entropy is that $\mathcal{S}$ is a single scalar value whose evolution condenses the required information on the spatial repartition. Moreover, as apparent from Eq. (1), the entropy $\mathcal{S}$ of the source distribution at generation g is bounded, namely,

$$0 \leqslant \mathcal{S}(g) \leqslant \log_2 B, \quad (2)$$

where B is the number of cells of the spatial mesh. This property ensures in particular that the variations of $\mathcal{S}$ will be bounded, and that the highest value of the entropy will be reached in the case of a perfect equipartition. The entropy function is nowadays a standard tool for most production Monte Carlo codes, although some concerns have been raised about possible issues related to its use in convergence diagnostics for loosely coupled multiplying systems (see, e.g., the analysis in Shi and Petrovic, 2010a,b; Ueki, 2005).

The latter issue with power iteration in Monte Carlo simulation concerns the impact of correlations induced by fission events: physically speaking, a neutron can only be generated in the presence of a parent particle, which induces generation-to-generation correlations (Lux and Koblinger, 1991; Sjenitzer and Hoogenboom, 2011). This is a widely recognized problem, which is expected to affect the convergence of Monte Carlo scores and in particular make the applicability of Central Limit Theorem questionable (Ueki, 2012; Brown, 2009; Ueki, 2005). Correlations between generations have been often studied within the mathematical framework provided by the eigenvalue analysis of the Boltzmann critical equation (Brown, 2005; Sutton, 2014a,b). Further work on correlations has concerned techniques aimed at improving the standard deviation estimates of Monte Carlo scores (Gelbard and Prael, 1990; Ueki et al., 2003, 2004; Dumonteil and Malvagi, 2012; Ueki, 2005). More recently, it has been pointed out that, due to the asymmetry between correlated births by fission and uncorrelated deaths by capture and leakage,[1] neutrons initially prepared at equilibrium will be preferentially found clustered close to each other after a few generations (Dumonteil et al., 2014). This peculiar phenomenon, named neutron clustering, might induce a strongly heterogeneous spatial repartition of the neutron population, which randomly evolves between generations (Dumonteil et al., 2014; Zoia et al., 2014; de Mulatier et al., 2015). The impact of neutron clustering has been determined to be inversely proportional to the number of neutrons per generation (Dumonteil et al., 2014).

In this paper, we will show that neutron clustering, not surprisingly, also affects the convergence of the fission sources: because of fission-induced correlations, the entropy function might in turn be ineffective at detecting potential deviations of the neutron population with respect to the expected equilibrium.

This manuscript is organized as follows. In Section 2, we will initially consider a simplified reactor model where exact analytical results can be established, and show that in some cases the convergence of the entropy is achieved, although the neutron population is still affected by strong spatial fluctuations. Then, in Section 3, we will refine our analysis based on the spatial moments of the entropy function and on the center of mass of the neutron population: these statistical tools can be used together with regular entropy so as to extract information concerning the simulated system, and thus improve the diagnosis of fission source equilibrium. In Section 4 we will then relate the behavior of such spatial fluctuations to the key system parameters, namely, the reactor size, the number of neutrons per generation, and the migration area, based on the theory of branching processes. In Section 5 we will numerically explore the behavior of a fuel rod and a full core with detailed geometry and compositions and continuous-energy treatment, and show that the theoretical findings for the simple reactor model actually apply more generally to realistic configurations. Conclusions will be drawn in Section 6.

2. Neutrons in a box and the behavior of the entropy

In order to assess the behavior of the entropy function in the presence of fission-induced correlations, we will work out an example that is simple enough for exact results to be analytically derived and compared to the Monte Carlo simulations, and yet retains the key physical features of a real system (Miao et al., 2016).

Let us therefore consider a prototype model of a reactor core consisting of a collection of N neutrons undergoing scattering, capture and fission within a box of volume $V = L^3$. To simplify the matter, we will assume that neutrons can only be reflected at the boundaries. The random displacements of the neutrons will be modeled by branching exponential flights with constant speed v; scattering and fission will be taken to be isotropic in the center of mass frame. The physical parameters of this prototype reactor will be the following:

$$\Sigma_s = 0.27, \quad \Sigma_c = 0.02, \quad \Sigma_f = \frac{\Sigma_c}{\bar{\nu} - 1.0}, \quad (3)$$

where Σ_s is the scattering cross section, Σ_c is the capture cross section, and Σ_f is the fission cross section (in cm^{-1}). The parameter $\bar{\nu}$ denotes the average number of secondary neutrons per fission. Observe that on the basis of the cross sections defined above the system is exactly critical, i.e.,

$$k_{eff} = \frac{\bar{\nu}\Sigma_f}{\Sigma_c + \Sigma_f} = 1, \quad (4)$$

for any choice of $\bar{\nu}$. For our simulations, we have set $\bar{\nu} = 2.5$. The fundamental eigenmode associated to $k_{eff} = 1$ corresponds to an equilibrium distribution that is spatially homogeneous over the box, as expected on physical grounds.

This prototype reactor model can be easily implemented and solved by power iteration within a Monte Carlo code. In order to probe the effects of neutron clustering on the convergence of power iteration, we have performed several Monte Carlo critical simulations of such system by varying the number N of particles per generation and the size L of the box, the other physical parameters being unchanged. For all configurations, we have assumed that the power iteration is started with a point source consisting of N neutrons located at the center of the box. As the number of generation increases, the neutron population spreads over the whole box, and is forced to converge towards the fundamental eigenmode by the power iteration. However, this spread is

[1] This phenomenon has been first investigated in the context of theoretical ecology, especially in relation to the evolution of biological communities: see, e.g., Young et al. (2001) and Houchmandzadeh (2008), and can be better understood in the framework of branching random walks (Athreya and Ney, 1972; Williams, 1974; Pázsit and Pál, 2008; Zoia et al., 2012).