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Clustering, Traveling Waves and Solitons in the Monte-Carlo Criticality Simulation of Decoupled and Confined Medium

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

I. INTRODUCTION

Monte-Carlo neutron transport codes [1, 2] are often used as 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 under-sampling effect biases the estimates of the variance of flux-based quantities [6, 7, 8, 9, 10]. Worse, in a work inspired by recent developments in population ecology [11, 12, 13, 14], Dumonteil, Mazzolo and Zoia have shown that non-Poisson spatial fluctuations were caused by a neutron clustering phenomenon [15, 16, 17, 18]: even for intermediate or high numbers of simulated neutrons, those fluctuations can make it hard to estimate flux-based standard deviations. In the present paper, we will show that space-dependent biases finding their origin in these spatial correlations also affect the estimates of flux-based quantities themselves, when leakage boundary conditions are employed. The first section will discuss the phenomenology of these biases on a commercial reactor benchmark, and on a simplified model grasping its main characteristics (the mass-preserved 1D binary branching Brownian motion on a segment with Dirichlet boundary conditions). In the second section we will build a functional equation modelling the simplified case, based on a generalized Fisher equation with time-dependent coefficients that allow for population control and that incorporates spatial correlations. In a third section, 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 have a soliton wave dynamic. 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 a last section.

II. BIASES ASSOCIATED TO THE MONTE-CARLO SIMULATION OF LARGE REACTOR CORES

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 other, 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 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, that depends on the spatial position of the tally volume [19, 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 Figure 1 and the associated "apparent" 1-σ error bars are provided by the left plot of Figure 2 (these error bars are calculated by the Monte Carlo code using the central limit theorem). As expected, the highest incertitudes 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 Figure 2 exhibit a spatial patterns: these errors seem to be big near the leaking boundaries of the reactor core but also close to the reflecting boundaries and at the center of the core. Such a non trivial spatial patterns is even more striking on the right plot of Figure 1, where the under-sampling 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 over-estimated near the leaking edges and is under-estimated at the center. In the following parts of this paper, we will try to model this very last phenomenon, also reported by many authors and papers.

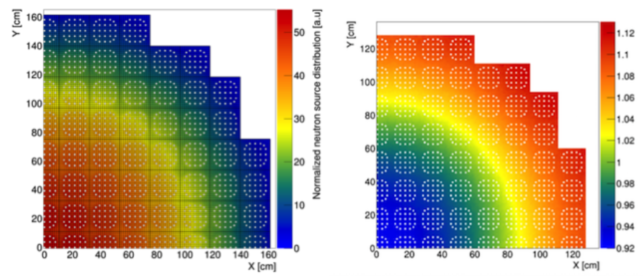

Fig. 1. MORET 5.B.2 simulation of the R1 OECD/NEA benchmark: axially averaged fluxes with 10^4 active cycles of 10^4 neutrons (left plot). Ratio of the axially averaged fluxes between a simulation with 10^6 active cycles of 10^2 neutrons and a simulation with 10^2 active cycles of 10^6 neutrons (right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

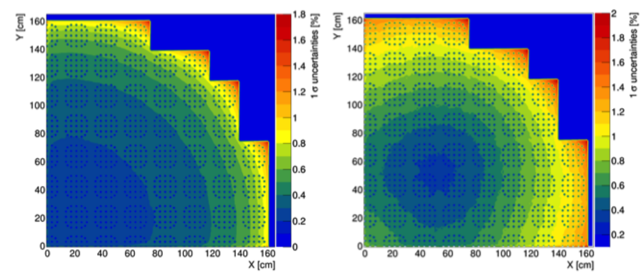

Fig. 2. MORET 5.B.2 simulation of the R1 benchmark with 10^4 active cycles of 10^4 neutrons: 1-σ error bars ("apparent errors") on the axially averaged fluxes (left plot) and 1-σ error bars ("true errors" estimated by independent simulations) on the axially averaged fluxes with 10^4 active cycles of 10^4 neutrons (right plot).

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, ...) so as 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 [24, 25, 26] on a segment (of half length L arbitrarily set to 20) with Dirichlet (leakage) boundary conditions allowed to observe precisely an under-estimation of the flux in the central region while reproducing an over-estimation of the flux close to the boundaries. The mass preserving mechanism is fully described Ref [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 splitted, 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 2-daughter particles fission cross-section β, and both were set to 0.1.Typical realization of such a process are provided Figure 3. As expected, this 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 strike one of the boundaries while wandering around, the constraint on the overall mass N of our mass-preserving process refrain 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 configurations, with dominant ratio sensitively less than 1), the splitting mechanism that compensates leakages picks particles according to a converged eigen-vector, and the bias disappear. Figure 4 sums up these discussions: the typical cosine-shape a one-group Boltzmann critical equation for a slab geometry is progressively distorted following a flat distribution at the center with a strong decay near the extremities, when the number of simulated particles gets smaller.

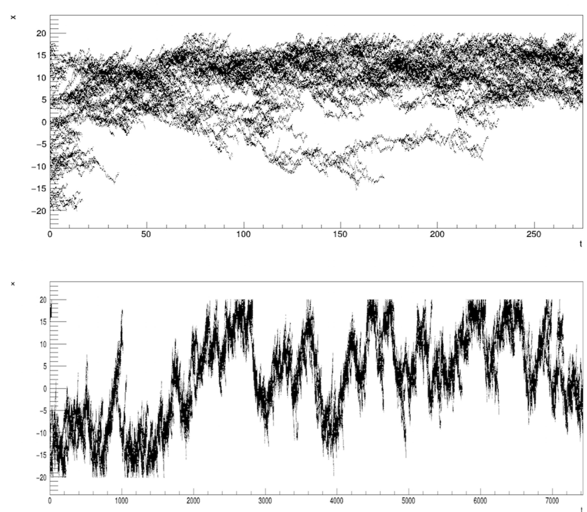

Fig. 3. x positions of the particles versus time t for 2 realisations of a mass-preserved binary branching Brownian motion on a segment (between -20 and 20) with Dirichlet boundary conditions and with $N = 50$ particles. Top plot: first realization observed between $t = 0$ and $t = 300$, bottom plot: second realization observed between $t = 0$ and $t = 7250$.

III. THE GENERALIZED FISHER EQUATION WITH POPULATION CONTROL

In this section we will build a stochastic model for our process (mass-preserved binary branching Brownian motion on a segment with Dirichlet boundary conditions) and discuss some of its analytical solutions, obtained under simplifying hypotheses.

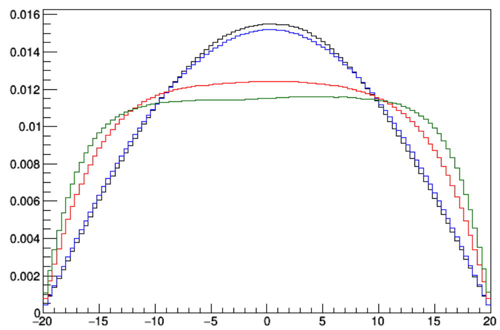

Fig. 4. Normalized particle density averaged over t=1000 (a.u.) for a mass-preserved binary branching Brownian motion on a segment (between -20 and 20) with Dirichlet boundary conditions and with N particles. Black curve: $N = 1000$, blue curve: $N = 100$, red curve: $N = 10$, green curve: $N = 5$.

1. Generalized Fisher equation

The key ingredient used as a starting point of our modeling is an adaptation of the Fisher equation [29, 30]. This equation is also known in population biology as the spatial logistic equation, or in theoretical physics as the KPP (Kolmogorov-Petrovsky-Piscounov) equation, and can be written

$$\partial_t \phi = D\nabla^2\phi + (\beta - \gamma)\,\phi + \lambda\,\phi^2, \tag{1}$$

where ϕ[1] is a density, D is the diffusion coefficient, β is a reproduction rate, γ is a disappearance rate and λ is a saturation rate. Depending on the sign of λ this saturation rate can be either a maximal threshold (for negative λ) or a minimal threshold (for positive λ). For example, in population ecology β and γ represent respectively the birth and death rates while λ might be interpreted as a saturation due to the competition for resources between individuals. Indeed this competition results from a local combinatorial interaction between the individuals, explaining that, at a given position, the death probability is adjusted by a saturation term. This term is proportional to the number of pair of individuals $\binom{N(x)}{2}$ in $x \pm dx$ (where $N(x) = \phi(x)dx$ is the number of individuals in $x \pm dx$), hence being quadratic in the ϕ-field.

When the competition term depends on the density of individuals, the clustering effect described Section I cannot be neglected anymore as it affects the density itself. Therefore the Poisson spatial distribution of individuals used to build Eq. (1) is no longer true and one have to resort to a generalized Fisher equation (see the pioneer work of *Birch et al* [31] for the full development). The generalized Fisher equation

$$\partial_t \phi = D\nabla^2\phi + (\beta - \gamma)\,\phi + \lambda \int dy\; \nu(|x-y|)\, G(x, y, t) \tag{2}$$

makes use of the pair correlation function G(x,y,t) which is defined such as $G(x, y, t)dxdy$ is the expected number of pair of individuals with one individual in x and the other in y, and of the competition kernel $\nu(r)$ that defines the spatial scale over which the competition occurs.

[1] In the following we will adopt a convention where the functions variables are implicit in order to lighten the equations. In this case, $\phi = \phi(x, t)$.

2. Time-dependent coefficients and population control

This generalized Fisher equation will now be adapted to reactor physics, so as to take into account different kind of feed-back effects that impose the overall number of neutrons to be constant such as:

- spatial and temporal control rod adjustments of the power which aim for instance at preventing local power excursion during the start-up phase of a reactor.
- the so-called "weight-watching" mechanism (Russian roulette and splitting) which are used at the end of each cycle (or each time step) of Monte-Carlo criticality (or dynamic) simulations to adjust the number of simulated neutrons to prevent any divergence or disappearance of the population. This mechanism is also referred to as the "renormalization" method in this context.

In neutron transport, the $\beta\phi$ and $\gamma\phi$ reaction rates now represent fission and capture events, and $\lambda \int dy\; \nu(|x-y|)\, G(x, y, t)$ describes in our case the rate at which local adjustment of the neutron density occurs in the general case where spatial correlations affect the population dynamics. In the following, and without loss of generality, we will keep in mind the Monte-Carlo criticality simulation of a 1-D branching Brownian with $k_{eff} < 1$: at each cycle (or similarly for any time), the number of neutrons produced by fission is smaller than the number of neutrons at the beginning of the cycle and the λ coefficient is therefore positive. It represents the splitting mechanism which produces neutron to compensate for leakages and absorptions. In this case, also, the competition kernel $\nu(r)$ can be simplified as the spatial range on which the population control is applied does not depend on the distance between neutrons: it is a global constraint on the overall population and will therefore be set to 1 in the following. Unfortunately, and as mentioned at the beginning of this sub-section, the local adjustments depend on time/generation: might it be for reactor core operation or for Monte-Carlo criticality simulation, the population number is constantly re-adjusted. In pretty much the same manner as in a work of *Newman et al* [32] we can therefore adjust the population by using a time dependant adjustment coefficient $\lambda(t)$. The population control criteria can be made explicit by integrating Eq. (2) over the positions between $-L$ and L which gives

$$\lambda(t) = \frac{-\beta + \gamma - D\int_{-L}^{L} dx\; \nabla^2\phi(x, t)}{\int_{-L}^{L} dx \int_{-L}^{L} dy\; G(x, y, t)}, \tag{3}$$

where we have used the following normalisation relation

$$\int_{-L}^{L} dx\; \phi(x, t) = 1. \tag{4}$$

In our example with $k_{eff} < 1$, this positive coefficient is interpreted as the splitting rate that compensates the neutron loss at each generation. It is consequently proportional to the number of captures (γ) and to the number of leakages

($-D\int_{-L}^{L} dx\, \nabla^2\phi(x,t)$) and is smaller when productions by fission (β) are important. Finally, it is more convenient to use the normalized and centered pair correlation function $g(x, y, t)$ defined as

$$g(x,y,t) = \frac{G(x,y,t) - \phi(x,t)\phi(y,t)}{\phi(x,t)\phi(y,t)}. \tag{5}$$

Upon injection in Eq. (2) we get our equation for the dynamic of a branching Brownian motion in a confined medium with population control

$$\begin{aligned} \partial_t\phi &= D\nabla^2\phi + (\beta-\gamma)\,\phi \\ &+\lambda(t)\left(1+\int_{-L}^{L} dy\; g(x,y,t)\phi(y,t)\right)\phi(x,t), \end{aligned} \tag{6}$$

with $\lambda(t)$ given by Eq. (3) and where we recall that $g(x, y, t)$ is the normalized and centered pair correlation function of our system.

IV. CLUSTERING AND TRAVELING WAVES IN BOUNDED DOMAINS

The rather intricate form of this generalized Fisher equation with population control does not allow for a direct solving all the more so, as the pair correlation function has not been made explicit. However, surprisingly enough, it is provided in a recent work of *De Mulatier et al* [18], where the authors were able to provide an amenable form of the correlation function for branching Brownian motion with population control on bounded domains. In this section we will therefore use an asymptotic analysis of Eq. (6), and we will show that its solution, in the case where the neutron population is small and whenever leakage boundary conditions are used, differs from the "deterministic" one, allowing to understand the cause and the structure of the bias observed section II.

1. Large population size

Whenever the neutron population N is very large, we have $g(x, y, t) \to 0$ as the spatial correlations arising from the branching process vanish (see for instance [31, 18]. Hence, the pair correlation function G becomes separable in x and y and we have $G(x, y, t) \to \phi(x, t)\phi(y, t)$ so that $\int dy\, G(x, y, t) \to \phi(x, t)$ and $\int dx \int dy\, G(x, y, t) \to 1$. The stationary limit of Eq. (6) takes in this case the very simple form

$$\nabla^2\phi - \left(\int_{-L}^{L} dx\, \nabla^2\phi(x)\right)\phi = 0. \tag{7}$$

Noticing that $\int_{-L}^{L} dx\, \nabla^2\phi(x) = \partial_x\phi(x)\big|_{x=\pm L}$, this equation simplifies to

$$\nabla^2\phi - \partial_x\phi(x)\big|_{x=\pm L}\,\phi = 0. \tag{8}$$

In the case of reflecting boundary conditions at each side of the domain, we have to use Neumann boundary conditions $\partial_x\phi\big|_{x=\pm L} = 0$. The equation Eq. (8) is therefore trivially verified, ensuring that the Monte-Carlo criticality renormalization in this case is unbiased.

In the case of absorbing boundary conditions at each side of the domain, we have to use Dirichlet boundary conditions given by $\phi(x,t)\big|_{x=\pm L} = 0$. Surprisingly enough, this boundary condition applied on a positive and symmetric function ensures that the coefficient in front of the term linear in ϕ is strictly positive. To go further, as a guess function it is possible to test the cosine solution of the diffusion approximation of the stationary Boltzmann critical equation with leakages. If we inject the test function $\phi(x) = A\, cos(\frac{\pi}{2}\frac{x}{L})$ (where A is an arbitrary constant) in Eq. (8), we have

$$\nabla^2\phi + \frac{\pi^2}{2L^2}\phi = 0. \tag{9}$$

The solution of this equation is indeed a cosine ensuring also that the Monte-Carlo criticality renormalization in this case is unbiased. Noticeable is the fact that none of the coefficients of this equation depend on the values of β, γ or D, and that there is always a solution to this problem, unlike for the critical diffusion equation where a criticality condition linking the geometry and the compositions has to be met. However this can be understood if we keep in mind that this is precisely the purpose of the renormalization: whatever the parameters characterizing the system, the simulation converges to an unbiased estimate of $\phi(x)$.

2. Small population size

If the neutron population N is too small, clusters of neutrons appear (see Refs. [16, 17, 18] for a precise criterium on N values that trigger the clustering phenomenon). For large time $t \to \infty$, only one cluster is still alive, with a constant number of neutrons N. This cluster wander around randomly, with a spatial extension determined by a normalized and centered correlation function that we call $g_N^\infty(x, y)$ and which analytical form is given Ref. [18]. Since we are interested in configurations triggering a strong clustering, it is safe to assume that $g_N^\infty(x, y) \gg 1$. This assumptions being valid whenever the renewal time $N/(\beta + \gamma + \lambda)$ is smaller than the mixing time $2L/D$, we can also conclude that the system size $2L$ has to be big, so that the dynamic of clusters far from the boundaries is the same whether we use Dirichlet or Neumann boundary conditions (leakages or reflections). We will therefore use the same correlation function for both conditions. Finally, for large time (one cluster) and systems having an important spatial extension, we can also assume that the correlation function only depends on $|x - y|$ so that $g_N^\infty(x, y) = g_N^\infty(|x - y|)$. Having all these assumptions in mind, the pair correlation function can be written

$$G(x,y,t) = g_N^\infty(|x-y|)\,\phi(x,t)\phi(y,t), \tag{10}$$

and its y-integral over the positions reads

$$\int_{-L}^{+L} dy\, G(x,y,t) = \phi(x,t)\int_{-L}^{+L} dy\; g_N^\infty(|x-y|)\phi(y,t), \tag{11}$$

Resorting to a similar development as exposed Ref. [31], this last expression takes the form

$$\int_{-L}^{+L} dy\, G(x,y,t) = \phi(x,t)\int_{-L}^{+L} g_N^\infty(|r|)dr\;\phi(x,t), \tag{12}$$

which transforms into

$$\int_{-L}^{+L} dy\, G(x,y,t) = g_N^\infty\, \phi(x,t)^2, \tag{13}$$

where we have defined $g_N^\infty = \int_{-L}^{+L} g_N^\infty(|r|)dr$. This allows to rewrite

$$\int_{-L}^{+L} dx \int_{-L}^{+L} dy\, G(x,y,t) = g_N^\infty \int_{-L}^{+L} dx\, \phi(x,t)^2, \tag{14}$$

so that Eq. (6) becomes

$$\partial_t\phi = D\nabla^2\phi + (\beta-\gamma)\,\phi + \left(\frac{-\beta+\gamma - D\,\partial_x\phi(x,t)\big|_{x=\pm L}}{\int_{-L}^{+L} dx \int_{-L}^{+L} dx\, \phi(x,t)^2}\right)\phi(x,t)^2. \tag{15}$$

When the cluster is far from the boundaries, the time-dependent coefficient in front of the ϕ^2 term becomes time-independent. Indeed, the leakages term can in this case be neglected and the normalization of the ϕ^2 term itself does not depend on time when t is big enough (the shape of the cluster is unchanged, as revealed by a careful analysis of the normalized pair correlation function [18]). In those conditions, preserving the normalization of the flux imposes $\int dx\, G(x,t) = 1$. We can therefore conclude that $\lambda(t) = \lambda = -(\beta-\gamma)$ so that our final equation is given by

$$\partial_t\phi = D\nabla^2\phi + (\beta-\gamma)\,\phi - (\beta-\gamma)\phi^2, \tag{16}$$

This traveling wave equation has been discussed Section III, and is even simpler in our case since both the linear and the quadratic terms in ϕ can be factorized

$$\partial_t\phi = D\nabla^2\phi + (\beta-\gamma)\,\phi(1-\phi). \tag{17}$$

It provides the full soliton dynamic of the neutron cluster. Written this way its meaning is straightforward: as soon as the flux exceeds a threshold ($\phi > 1 = \int dx\, \phi$), the population control counteracts by russian roulette to maintain the fixed size of the population. When the flux gets too small, the splitting of neutrons induces an artificial fission process in the same aim. Since the spatial correlation function of the cluster is unchanged, the neutron cluster behaves like a soliton wave, just like observed Figure 3. By integration over time, the density profile of the flux can also be retrieved and presents a flat structure.

Indeed, a numerical time-integration of this equation together with its limit condition $\phi(\pm L) = 0$, is given Figure 5. In particular, its stationary shape is very close to the one simulated Figure 4 with very few number of neutrons.

It is also important to notice that this mean field equation has a different form than the cosine shape solution of the one-group criticality diffusion equation, explaining thus qualitatively the biases observed Figure 4. This can nicely be interpreted as follows: far from the boundaries, the soliton wave of our cluster averages so as to produce a flat density profile. Near the boundaries, the leakages are big and are therefore compensated by a very strong splitting of neutrons required to keep the overall mass constant. This produces a reflection of the whole wave on the boundary, explaining thus that the lower the number of neutrons, the flatter the distribution (even near the edges of our system).

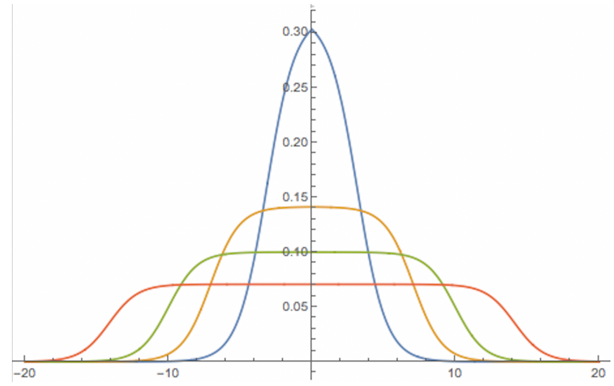

Fig. 5. Normalized particle density as a function of the position x given by a numerical integration of Eq. (17) ($D = 1$, $\gamma = 1$, $\beta = 0$ and initial Dirac delta function source) up to different observation time (from the blue curve to the red curve as time goes by). As time goes by, the neutron population explores the available space until it reaches the boundaries of the domain and stabilizes.

V. CONCLUSIONS

By resorting to a generalized Fisher-like equation with time-dependent coefficients that allows for population control, we have successfully built a stochastic modeling able to reproduce under-sampling biases observed in the Monte Carlo criticality simulation of loosely coupled systems and large reactor cores. An asymptotic analysis of this equation made it possible to study the dynamics of clustered population of neutron, and we have shown that it obeys a soliton wave equation, while the flux profile is governed by a traveling wave equation. We have also shown in particular that the biases arising in Monte-Carlo criticality simulation of decoupled systems can be understood as arising from spatial correlations and neutron clustering combined with leakage boundary conditions. In a future work we will present a variance reduction scheme that allows to deal with this clustering effect, in order to get rid of the under-sampling bias.

VI. ACKNOWLEDGMENTS

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