The criticality of multiplicative processes

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Abstract

Keeping in view applications to numerical simulations of the evolution of a nuclear reactor core around criticality, we use a general mathematical framework for describing the evolutions of multiplicative processes (processes involving particle creation) both in particle generations and in time. This framework allows us to obtain, within a same formalism, two corresponding estimates of the multiplication factor which describes the growth of particle numbers at large times. We obtain the relative positions of both estimates with respect to each other and to criticality. These relations may show particularly useful when simulating in a realistic way the monitoring of nuclear cores in subcritical states, such as is the case for Accelerator Driven Systems (ADS). More generally, this study applies to various multiplicative processes which can be found in nature.
I. INTRODUCTION

The development of new designs represents an important challenge for the future of nuclear energy production. The complexity of the physics involved and the strong constraints imposed by practical realizations, in particular security issues, imply that the approaches dedicated to the development of original designs heavily rely on modelizations and simulations and that the latter must be made as faithful as possible. Simulations appear crucial for studying the feasibility of innovative designs mixing different technologies. Such is the case in particular of Accelerator Driven Systems (ADS) which associate a nuclear core, which burns a fissile material, with a proton source, producing by spallation the neutrons which initiate the nuclear reactions chains [1–3]. Characteristic features of these systems, which play an important role with respect to security issues, are their operation below criticality and the ability to monitor their power using the proton source [4, 5].

In an approach which is commonly used to develop models and simulations of nuclear cores and to study their properties with respect to criticality, one focuses on the behavior of averaged neutron fluxes at large time scales [6]. Such an approach is well suited to the study of the neutronic evolution of homogeneous nuclear cores in quasi stationary states, such as those building the nuclear plants which are operated for power production. This shows particularly useful when studying power production, fissile material regeneration or fission products accumulation on a long term. In that case, criticality refers to the multiplicative character of the averaged neutron flux over the whole core, and is represented by a multiplication factor (equivalently, by a $k_{\text{eff}}$ coefficient). The latter, which characterizes the global state of the nuclear core at large time scales, can be obtained in Monte Carlo simulations as the largest eigenvalue of a time independent matrix describing the effect of fissions on successive generations of neutrons within the nuclear core [6, 7].

In the case of ADS however, one must consider the correlated time evolutions of the different elements composing the core, paying attention to the spatial distributions of neutron fluxes and matter contents. Simulations with a time specific approach appear to be necessary [8, 9], as the transient properties of neutron fluxes and the position of the spallation source relative to the nuclear core now play an important role. This is exhibited in experimental ADS, where measurements of neutron fluxes show that the properties of the proton source
used for producing spallation neutrons strongly influence the time and spatial distributions of neutrons within the core [10]. In general, an approach with an explicit time dependence may be required, for instance when assessing the effect of security devices or when studying the impact of the proton source on the critical properties of the nuclear core [11, 12]. In that case, the time evolution of neutron fluxes is better described by a time evolution operator acting on spatial densities. The multiplication factor characterizing the growth of neutron fluxes is defined from this time evolution operator. The question then arises of relating the corresponding properties of neutron fluxes, which can be locally measured, to the parameters which characterize the global state of the nuclear core in a time independent way, in particular with respect to criticality [12].

Due to intrinsic complexities, the generation and the time dependent approaches are usually not followed simultaneously within a same formalism. This constitutes a drawback for modelizations and simulations of the time monitoring of nuclear cores, close to criticality and with significant spatial inhomogeneities as in ADS. In particular, ambiguities arise when trying to relate kinetic parameters, which characterize the global state of the nuclear core and which can be obtained from Monte Carlo simulations, to experimental measurements performed on neutron fluxes at chosen locations [10, 12]. These difficulties show to be critical when trying to assess the efficiency of security devices, such as absorber bars, or when studying the consequences of a power breakdown in ADS. In such cases, a bridge between the different approaches would be much helpful, as it would allow one to compare the kinetic parameters, like the multiplication factor, which are obtained from different types of simulations and to apply these results to experimental situations.

The fundamental processes occurring in a nuclear reactor may be characterized as multiplicative processes, i.e. processes involving particle creation, hence numbers of particles which vary in time. These fundamental processes, although characterized by cross-sections which slowly vary in time, build the nuclear reaction chains which, together with the system geometry, ultimately determine the global parameters characterizing the system (produced power, neutron fluxes, matter contents, ...), which become time dependent. Simulations, either in deterministic or Monte Carlo approaches, rely on numerical computations and hence require discretized representations of time and space, under the form of an elementary time interval, or time step, and elementary space cells. The errors induced by this discretization,
both statistically and systematically, are controlled to a required level of precision by diminishing the sizes of the elementary time step and space cells. The resulting increase in computation time is ultimately limited by available computing capacities. The important improvement in velocity and memory capacities reached by computers in the last decades has significantly increased the precision attainable by simulations. But present simulation codes still need to be strongly optimized in order to reach the sensitivity level allowing a comparison with experimental measurements. Simulating systems at very low subcriticality even requires too small time steps to allow one to satisfactorily estimate the corresponding multiplication factor. The situation is even more critical for ADS, as optimization leads to adopting different time steps for describing the evolutions of different parts of the system (proton source, nuclear core), thus entailing tradeoffs which may significantly affect the precision which can be reached.

When focusing on the large time behavior of a nuclear core, these difficulties can be circumvented in Monte Carlo simulations by using the generation approach, that is by generating neutrons according to some characteristics and by following all particles (including neutrons and fission products), which are successively generated by interacting with the different materials building the nuclear core. Parameters like the multiplication factor are then deduced from a transfer matrix, representing the evolution of the system along successive generations of neutrons, without relying on an explicit time step dependence\textsuperscript{7}. Nevertheless, the nature of the simulation code still allows one to recover time dependencies, at the expense of degrading the precision level. The same approach can be applied to ADS and, near criticality, the different time steps may be optimized so that to allow one to obtain some time dependent parameters with a satisfactory precision level. It should then become feasible to compare the estimations of the kinetic parameters which are given by the generation and the time dependent approaches.

The multiplication factor (or equivalently the $k_{\text{eff}}$ coefficient), which is used to characterize the global state of a system with respect to criticality, plays a crucial role when addressing safety and efficiency issues. As two different estimates can be given of the multiplication factor, that is, according to the generation approach or to the time dependent approach, it becomes important to determine their relative positions with respect to each other and with respect to criticality. The aim of this article is to follow both approaches
simultaneously within a same formalism, and hence to prove that both estimates of the multiplication factor can be used equivalently near criticality and, more precisely, to determine their relative positions in a rigorous way.

The formalism which is used here is the one underlying Monte Carlo simulations, i.e. the Master equation approach. This formalism appears in non-equilibrium statistical mechanics in order to describe the evolution of many body systems [13–16]. It is very briefly presented in section 2, together with the processes which are specific to nuclear reactors (absorption, diffusion, fission). The equation describing the time evolution of averaged numbers of particles is deduced. In this approach, time is discretized, as well as the particles phase space. In section 3, generations of particles are defined: initially, all particles belong to generation 0 until the first creation event, after which they belong to generation 1, etc... The generation evolution equation is given by a matrix with non negative elements, for which the Perron-Frobenius theorem applies [17], insuring the existence of a highest positive eigenvalue controlling the spectrum of the matrix. Generation criticality is defined in terms of this eigenvalue in section 4. Both definitions of criticality (in terms of time evolution and of generation evolution) are then proved to be equivalent. The behavior around criticality is also studied in this section.

II. MULTIPLICATIVE PROCESSES

In this section, we first present the basic definitions and the assumptions which allow one to apply the Master equation approach to the time evolution of multiplicative processes, in the context of discretized time and phase space. Specifying the different elementary processes affecting a neutron in a nuclear reactor core, one then applies the Master equation approach to the description of neutron densities within the core and obtains the equations which describe the time evolution of the numbers of neutrons in the different elementary cells.

A. Cells and configurations

We consider a finite set \( A \), with elements denoted by \( \alpha, \beta, \ldots \in A \). An element of \( A \) will be called a cell. A configuration is the data of the occupation numbers \( \{n_\alpha\} \) of the cells \( \alpha \),
where \( n_\alpha \) is a positive integer, the number of particles in cell \( \alpha \). We consider a stochastic process \( \{ N_\alpha(t) \} \) associated with the evolution of occupation numbers \( \{ n_\alpha \} \) in time \( t \) and define the corresponding probability

\[
P(\{n_\alpha\}, t) \equiv \text{Prob}\{N_\alpha(t) = n_\alpha, \forall \alpha \in A\}
\]

The time variable \( t \) is either discrete or continuous. In the former case, a time step \( \Delta t \) is chosen and fixed once for all. To take into account the initial configuration \( \{ n_\alpha(0) \} \), we define the conditional probability

\[
P(\{n_\alpha\}, t|\{n_\alpha(0)\}) \equiv \text{Prob}\{N_\alpha(t) = n_\alpha, \forall \alpha \in A|N_\alpha(0) = n_\alpha(0), \forall \alpha \in A\}
\]

We shall use the obvious convention \( P(\{n_\alpha\}, t) = 0 \) if one of the \( n_\alpha \) is strictly negative.

### B. Elementary processes

We define a multiplicative stochastic process \( \{ N_\alpha \} \) in discrete time as a Markov process with transition probabilities in one time step

\[
\text{Prob}\{\{N_\alpha(t+\Delta t)\} = \{n'_\alpha\}|\{N_\alpha(t)\} = \{n_\alpha\}\} \equiv R(\{n'_\alpha\}|\{n_\alpha\})
\]

which satisfies the following conditions:

(i) we assume that the various particles (belonging to the same or different cells) do not interact with each other, i.e. are independent. As a consequence, it is sufficient to specify the transition probabilities of the elementary processes in one time step for a given particle in a given cell \( \beta \) (for every \( \beta \))

(ii) we define \( R(\{q_\alpha\}|\beta) \) the probability that a particle in cell \( \beta \) at time \( t \) creates, at time \( t + \Delta t \), \( q_\alpha \) particles in the cell \( \alpha \), for all \( \alpha \). \( \{q_\alpha\} \) is a collection of integers which are positive for \( \alpha \neq \beta \) and \( \geq -1 \) for \( \alpha = \beta \) (destruction of one particle in \( \beta \) and possible creation of particles in \( \beta \)). We assume that, if \( \{q_\alpha\} \neq \{0\} \) i.e. at least one particle is created in some cell or destroyed in \( \beta \), the quantities \( R \) are proportional to \( \Delta t \)

\[
R(\{q_\alpha\}|\beta) \equiv \hat{R}(\{q_\alpha\}|\beta)\Delta t, \quad \text{for} \quad \{q_\alpha\} \neq \{0\}
\]

(iii) we assume that the probability that a particle in cell \( \beta \) does not create any new particle and is not destroyed is a positive quantity, defined by

\[
R(\{0\}|\beta) \equiv 1 - \sum_{\{q_\alpha\} \neq \{0\}} R(\{q_\alpha\}|\beta)
\]
Hence, the transition probabilities in one time step $R(\{n'_\alpha\}|\{n_\alpha\})$ between a configuration $\{n_\alpha\}$ at time $t$ and a configuration $\{n'_\alpha\}$ at time $t+\Delta t$ for the stochastic process $\{N_\alpha\}$ are specified by

$$R(\{n_\alpha + q_\alpha\}|\{n_\alpha\}) \equiv \sum_\beta R(\{q_\alpha\}|\beta)n_\beta, \quad \text{if} \quad \{q_\alpha\} \neq \{0\}$$

$$R(\{n_\alpha\}|\{n_\alpha\}) \equiv 1 - \sum_{\{q_\gamma\} \neq \{0\}} R(\{q_\gamma\}|\beta)n_\beta$$

(6)

C. Master equation and equations for the moments

The evolution of the probability $P(\{n_\alpha\})$ (equation (1)) is given in discrete time by the transition probability (3) and equations (6)

$$P(\{n_\alpha\}, t+\Delta t) = \left(1 - \sum_{\{q_\gamma\} \neq \{0\}} R(\{q_\gamma\}|\beta)n_\beta\right) P(\{n_\alpha\}, t)$$

$$+ \sum_{\{q_\gamma\} \neq \{0\}} R(\{q_\gamma\}|\beta)(n_\beta - q_\beta)P(\{n_\beta - q_\beta\}, t)$$

(7)

(with $P(\{n_\alpha\}) = 0$ as soon as $n_\alpha < 0$ for one $\alpha$).

For each cell $\alpha \in A$ the mean occupation number $\bar{n}_\alpha(t)$ and its correlations $c_{\alpha,\beta}(t)$ are defined by

$$\bar{n}_\alpha(t) \equiv <N_\alpha(t)> \equiv \sum_{\{n_\gamma\}} n_\alpha P(\{n_\gamma\})$$

$$\bar{n}_{\alpha,\beta}(t) \equiv <N_\alpha(t)N_\beta(t)> \equiv \sum_{\{n_\gamma\}} n_\alpha n_\beta P(\{n_\gamma\})$$

$$c_{\alpha,\beta}(t) \equiv \bar{n}_{\alpha,\beta}(t) - \bar{n}_\alpha(t)\bar{n}_\beta(t)$$

(8)

The evolution equations for the mean occupation number and its correlations are deduced
from the master equation (7)

\[
\bar{n}_\alpha(t + \Delta t) = \bar{n}_\alpha(t) + \sum_{\{q_\gamma\},\beta} R(\{q_\gamma\}|\beta) q_\alpha \bar{n}_\beta(t)
\]

\[
\bar{n}_{\alpha,\beta}(t + \Delta t) = \bar{n}_{\alpha,\beta}(t) + \sum_{\{q_\gamma\},\delta} R(\{q_\gamma\}|\delta) (q_\alpha q_\beta \bar{n}_\delta(t) + q_\alpha \bar{n}_{\beta,\delta}(t) + q_\beta \bar{n}_{\alpha,\delta}(t))
\]

\[
c_{\alpha,\beta}(t + \Delta t) = c_{\alpha,\beta}(t) + \sum_{\{q_\gamma\},\delta} R(\{q_\gamma\}|\delta) (q_\alpha q_\beta \bar{n}_\delta(t) + q_\alpha c_{\beta,\delta}(t) + q_\beta c_{\alpha,\delta}(t))
\]

\[
- \left( \sum_{\{q_\gamma\},\delta} R(\{q_\gamma\}|\delta) q_\alpha \bar{n}_\delta(t) \right) \left( \sum_{\{q_\gamma\},\delta} R(\{q_\gamma\}|\delta) q_\beta \bar{n}_\delta(t) \right)
\] (9)

Let us remark that closed equations (9) have been obtained for the first and second moments of the random variable \(N_\alpha(t)\). This is due to the fact that the particles do not interact with each other, so that the transition probability in the master equation depends linearly on the number of particles (see [7]).

D. Specification of elementary processes

From now on, the particle will be assumed to undergo one of the following elementary processes:

(i) Absorption

In this case, a particle in cell \(\beta\) is absorbed (and then disappears) in one time step, so that \(q_\beta = -1\) and \(q_\alpha = 0\) for \(\alpha \neq \beta\). The probability for absorption will be denoted by \(A_\beta\)

\[
R^{\text{absorption}}(\{q_\alpha\}|\beta) \equiv A_\beta \prod_\alpha \delta(q_\alpha + \delta_{\alpha\beta})
\] (10)

(ii) Diffusion

In this case, a particle in cell \(\beta\) is transmitted to a cell \(\gamma \neq \beta\), so that \(q_\gamma = 1, q_\beta = -1\) and \(q_\alpha = 0\) for \(\alpha \neq \beta\) and \(\alpha \neq \gamma\). The probability for diffusion will be denoted by \(D_{\gamma\beta}\)

\[
R^{\text{diffusion}}(\{q_\alpha\}|\beta) \equiv D_{\gamma\beta} \prod_\alpha \delta(q_\alpha + \delta_{\alpha\beta} - \delta_{\alpha\gamma}), \quad D_{\beta\beta} \equiv 0
\] (11)

(iii) Fission

In this case, a particle in cell \(\beta\) creates \(q_\alpha \geq 0\) particles in cell \(\alpha\) in one time step with \(\sum_{\alpha \in A} q_\alpha > 0\), so that one has net creation. Moreover, either \(q_\beta = -1\) (the particle in destroyed during the fission process) or \(q_\beta \geq 0\) (the particle in cell \(\beta\) is recreated during the
fission process together with other particles). The probability for fission will be denoted by \( F(\{q_\alpha\}|\beta) \)

\[
R^{\text{fission}}(\{q_\alpha\}|\beta) \equiv F(\{q_\alpha\}|\beta), \quad F(\{0\}|\beta) \equiv 0 \quad (12)
\]

(iv) Nothing

The probability that a particle in cell \( \beta \) remains in cell \( \beta \) doing nothing in one time step is thus (the sum of the probabilities of processes (i), (ii), (iii) and (iv) must be 1)

\[
R^{\text{nothing}}(\{q_\alpha\}|\beta) \equiv R(\{0\}|\beta) \prod_\alpha \delta(q_\alpha)
\]

\[
R(\{0\}|\beta) = 1 - A_\beta - \sum_\gamma D_{\gamma\beta} - \sum_{\{q_\gamma\}} F(\{q_\gamma\}|\beta) \quad (13)
\]

This last quantity is assumed to be positive and \( A, D \) and \( F \) to be proportional to the time step \( \Delta t \), which should be a small quantity, so that (13) will be close to 1 for small \( \Delta t \). Finally, we denote by \( R \) the substochastic matrix defined by

\[
R_{\alpha\beta} \equiv \sum_{\{q_\gamma\}} (R^{\text{absorption}}(\{q_\gamma\}|\beta) + R^{\text{diffusion}}(\{q_\gamma\}|\beta) + R^{\text{nothing}}(\{q_\gamma\}|\beta)) q_\alpha
\]

\[
+ \delta_{\alpha\beta} (1 - \sum_{\{q_\gamma\}} R^{\text{fission}}(\{q_\gamma\}|\beta))
\]

\[
= D_{\alpha\beta} + R(\{0\}|\beta) \delta_{\alpha\beta}
\]

\[
\sum_\alpha R_{\alpha\beta} \leq 1 \quad (14)
\]

Then, \( R_{\alpha\beta} \) describes the probability for a particle in a cell \( \beta \) to diffuse to another cell \( \alpha \) or to stay in the same cell \( \beta \) without doing anything (absorption or fission).

The time evolution of the mean occupation number (9) may then be rewritten in terms of a matrix \( S \) defined by

\[
\bar{n}_\alpha(t + \Delta t) = \sum_\beta S_{\alpha\beta} \bar{n}_\beta(t)
\]

\[
S_{\alpha\beta} \equiv \delta_{\alpha\beta} + \sum_{\{q_\gamma\}} R(\{q_\gamma\}|\beta) q_\alpha = R_{\alpha\beta} + F_{\alpha\beta}
\]

\[
F_{\alpha\beta} \equiv \sum_{\{q_\gamma\}} (q_\alpha + \delta_{\alpha\beta}) F(\{q_\gamma\}|\beta) \quad (15)
\]

Then, \( F_{\alpha\beta} \) describes the mean number of particles produced by fission in a cell \( \alpha \), in one time step, by a particle originating from a cell \( \beta \). The second term in the fission matrix \( F \)
takes into account the fact that a particle destroyed by fission in a cell \( \beta \) recreates \( q_\beta + 1 \) particles if they are produced in the same cell \( \beta \) (the diagonal part of the matrix \( R \) accounts for the destruction of one particle in cell \( \beta \)).

The time evolution of the second moment \((9)\) may similarly be rewritten in terms of the matrix \( S \)

\[
\bar{n}_{\alpha,\beta}(t + \Delta t) = \sum_{\gamma,\delta} \left( S_{\alpha,\gamma} \delta_{\beta,\delta} + S_{\beta,\gamma} \delta_{\alpha,\delta} - \delta_{\alpha,\gamma} \delta_{\beta,\delta} \right) \bar{n}_{\gamma,\delta}(t) + \sum_{\{q_\gamma\},\delta} R(\{q_\gamma\}|\delta) q_\alpha q_\beta \bar{n}_\delta(t)
\]  

(16)

Note that the time step \( \Delta t \) is constrained by the positivity of the probability \( R_{\alpha,\beta} \)

\[
0 \leq R(\{0\}|\beta) \leq 1 \quad \Rightarrow \quad 0 \leq \Delta t \leq \frac{1}{\max_{\beta} \left( \dot{A}_\beta + \sum_{\gamma} \dot{D}_{\gamma,\beta} + \sum_{\{q_\gamma\}} \dot{F}(\{q_\gamma\}|\beta) \right)}
\]  

(17)

Equations (15) are the main result of this section. They explicitly give the time evolution of the spatial distribution of neutrons once the cross sections of the elementary processes affecting neutrons in the reactor nuclear core are known. The latter, together with the system geometry, i.e. the definition and matter contents of the elementary cells, completely determine the matrix \( S \), which summarizes the probabilities of the elementary processes occurring in each cell.

III. EVOLUTION OF GENERATIONS

In this section, we define the notion of generation for multiplicative processes and the transfer matrix \( T \) describing the corresponding evolution equation. We also obtain the relation between the two matrices, respectively \( S \) and \( T \), which describe the evolution of the system with respect to time and generations respectively.

A. Generations

Suppose that at time \( t = 0 \) a configuration \( \{n^{(0)}_\alpha\} \) is given. The particles of this configuration will be called particles of generation 0. Let \( \{N_\alpha\} \ (t \equiv k\Delta t, \ k \ \text{integer}) \) the stochastic process starting from \( \{n^{(0)}_\alpha\} \). We consider a given particle of generation 0 at time \( t = 0 \) and
follow it until it produces a fission event: the particles which are produced at this fission event are called particles of first generation. Let \( n_1(\alpha) \) the number of particles of first generation produced in cell \( \alpha \) by the particles of generation 0. Clearly, these particles are not produced at the same time. It can also happen that a particle of generation 0 is absorbed before producing any fission event, so that it produces no particle of generation 1.

We define recursively \( n_i(\alpha) \) as the number of particles of generation \( i \) produced (by fission) in a cell \( \alpha \). We consider the fission event (if any) produced by a particle of generation \( i \) at some time. This fission event produces particles in various cells which are called particles of generation \( i+1 \). The total number of particles of generation \( i+1 \) in a cell \( \alpha \) will be denoted by \( n_{i+1}(\alpha) \). By definition also, \( n_0(\alpha) \equiv n_0^{(0)}(\alpha) \).

Let \( T_i(\alpha|\beta) \) be the number of particles of generation \( i \) produced in a cell \( \alpha \) by a single particle of generation 0 in cell \( \beta \). The matrix \( T \) with elements \( T_1(\alpha|\beta) \) will be called the generation transfer matrix. It may be that \( T_i(\alpha|\beta) \) is 0, but it is also clear that

\[
n_i(\alpha) = \sum_\beta T_i(\alpha|\beta)n_0(\beta)
\]

\[
T_i(\alpha|\beta) = (T^i)_{\alpha\beta}
\]

One also has for one generation step

\[
n_{i+1}(\alpha) = \sum_\beta T_{\alpha\beta}n_i(\beta)
\]

which is the evolution equation for generations.

**B. Transfer matrix for generations**

If a particle starts at time \( t = 0 \) in cell \( \beta \), the probability that in \( n \) time steps it propagates to a cell \( \alpha \) (or stays in \( \beta \) if \( \alpha = \beta \)), without being absorbed or producing fission, is given by \( (R^n)_{\alpha\beta} \) where \( R \) is the matrix defined in equation (14). Then, the probability that a particle propagates in any time steps from a cell \( \beta \) to a cell \( \alpha \) without being absorbed or producing fission is given by \( (\sum_{n=0}^{\infty} R^n)_{\alpha\beta} = \left( \frac{1}{1-R} \right)_{\alpha\beta} \). Then, the element \( T_{\alpha\beta} \) of the generation transfer matrix, i.e. the mean number of particles produced in a cell \( \alpha \) by a particle originating from a cell \( \beta \), is given by

\[
T_{\alpha\beta} = (F \frac{1}{1-R})_{\alpha\beta}
\]
Relation (20) for the generation transfer matrix may also be obtained from the following reasoning. In one time step, a particle in a cell $\beta$ either diffuses to a cell $\alpha$ without producing fission, with probability $R_{\alpha\beta}$, or produces $q_\alpha$ particles ($q_\beta + 1$ if $\alpha = \beta$) by fission with probability $F$($\{q_\alpha\}$|$\beta$) (see (15)). Then, a particle of a given generation in a cell $\alpha$ either comes from a particle of the same generation from another cell $\gamma$ or has been produced by fission in $\alpha$. So that the number of particles $T_{\alpha\beta}$ produced by fission in cell $\alpha$ by a particle from a cell $\beta$ must satisfy

$$T_{\alpha\beta} = \sum_\gamma T_{\alpha\gamma} R_{\gamma\beta} + F_{\alpha\beta}$$

$$\Leftrightarrow T = F \frac{1}{1 - R}$$

(21)

$1 - R$ must be invertible for relation (20) to make sense. We briefly show that this is the case when the matrix $R$ is irreducible, due its definition (14). From the definition (14), one has $\sum_\alpha R_{\alpha\beta} = 1 - A_\beta - \sum_{\{q_\gamma\}} F$($\{q_\gamma\}$|$\beta$) $\leq 1$ and assuming that there is at least one absorption or fission process, one deduces that there is at least one $\beta$ for which $\sum_\alpha R_{\alpha\beta} < 1$. Assuming that $R$ is irreducible ($\forall \gamma, \delta, \exists n : (R^n)_{\gamma\delta} \neq 0$), there follows that the strict inequality holds for every element $\gamma \in A$ for some $R^n$ ($\forall \gamma \in A, \exists n : \sum_\alpha (R^n)_{\alpha\gamma} \leq \sum_\alpha R_{\alpha\beta} < 1$). But then, $R$ cannot have 1 as an eigenvalue. For in that case, the corresponding left eigenvector $u$ would satisfy contradictory properties

$$\bar{\alpha} : |u_{\bar{\alpha}}| \equiv \max_{\alpha} |u_\alpha|$$

$$|u_{\bar{\alpha}}| = |\sum_{\alpha} u_\alpha (R^n)_{\alpha\bar{\alpha}}| \leq \max_{\alpha} |u_\alpha| (\sum_{\alpha} (R^n)_{\alpha\bar{\alpha}}) < \max_{\alpha} |u_\alpha|$$

(22)

Relation (20) shows that the generation transfer matrix corresponds to a partial resummation of the time evolution, $R^n$ corresponding to the free evolution of a particle in $n$ time steps. The partial re-summation provides equations which extend the time evolution equations (15) beyond the perturbative regime (in $\Delta t$). Indeed, while the probabilities of elementary processes are of the order of the time step $\Delta t$, which is bounded according to equation (17), in contrast the generation transfer matrix is of order 1

$$R \equiv 1 + \dot{R} \Delta t + O(\Delta t^2), \quad F \equiv \dot{F} \Delta t + O(\Delta t^2)$$

$$T = F \sum_{n=0}^{\infty} (\dot{R} \Delta t)^n = \frac{-\dot{F}}{\dot{R}} + O(\Delta t)$$

(23)
The following relation holds between the time evolution matrix $S$ and the generation transfer matrix $T$

$$S = R + F = 1 - (1 - T)(1 - R) \tag{24}$$

Relation (24) constitutes the main result of this section. It allows one to compare the evolutions of the system, either in time, with the matrix $S$, or in generations with the transfer matrix $T$. Let us note that, whatever the transfer matrix $T$, the time evolution matrix $S$ always remains close to 1 for small time step $\Delta t$.

IV. CRITICALITY

In this section, we define the multiplication factors which can be associated with the evolution matrices $S$ and $T$, and derive the relation connecting these two definitions, using relation (24) between matrices $S$ and $T$. We also derive a more explicit expression for this relation close to criticality.

A. Notations

Let $M$ be a matrix with positive elements. According to Perron-Frobenius theorem, there exists an eigenvalue $\lambda_M > 0$ with an eigenvector with positive components, such that all eigenvalues $\lambda_r$ of $M$ are complex numbers with $|\lambda_r| \leq \lambda_M$. If $M$ is irreducible, in the sense that $M^n$ has all elements strictly positive for $n$ large enough, $\lambda_M$ is non degenerate and its eigenvector has all its components strictly positive. Moreover, the eigenvalue $\lambda_M$ is given by

$$\lambda_M = \max_{v > 0} \min_k \frac{(Mv)_k}{v_k}, \quad (v > 0 \iff v_k > 0, \forall k) \tag{25}$$

For a stochastic matrix $M$ (i.e. $\sum_k M_{kl} = 1, \forall l$), then $\lambda_M = 1$.

Eigenvalues of the matrix $M$ will be arranged by decreasing order of moduli $\lambda_M \equiv \lambda_O > |\lambda_1| \geq ... \geq |\lambda_n|$ and left and right eigenvectors with eigenvalue $\lambda_r$ will be denoted by $u^r(M)$ and $v^r(M)$ respectively and normalized according to $\sum_k u^r_k v^r_k = 1$, so that powers of $M$ will read $M^n_{kl} = \sum_r \lambda^n_r u^r_k v^r_l$. 

13
B. Criteria for criticality

Two a priori different notions of criticality may be given for a multiplicative process. The first one depends on the time evolution of the mean occupation number \( \langle n \rangle \) while the second one depends on the evolution of generations \( I \). The large time asymptotics for the solution of the time evolution equation for the mean occupation number and for the generation number respectively give

\[
\bar{n}_\alpha(N\Delta t) \simeq \lambda_S^N u_\alpha^0(S)\left(\sum_\gamma v_\gamma^0(S)\bar{n}_\gamma^{(0)}\right), \quad \text{for} \quad N \gg 1
\]

\[
n_I(\alpha) \simeq \lambda_T^I u_\alpha^0(T)\left(\sum_\gamma v_\gamma^0(T)\bar{n}_\gamma^{(0)}\right), \quad \text{for} \quad I \gg 1
\]  

Recall that criticality is defined as the condition for stationarity of particle numbers at large time, \( \lambda_S = 1 \) or \( \lambda_T = 1 \). Hence, \( \lambda_S < 1 \) (resp. \( \lambda_S > 1 \)) or \( \lambda_T < 1 \) (resp. \( \lambda_T > 1 \)) correspond to subcriticality (resp. supercriticality). Two different criteria for criticality are thus obtained, according to the largest eigenvalue \( \lambda_S \) or \( \lambda_T \) which is chosen for discussing the asymptotic behavior of particle numbers.

One must note a fundamental difference between the two criteria. The first criterion relies on a comparison between two time scales, a small one \( \Delta t \) (see (17)), necessary to define the infinitesimal probabilities (proportional to \( \Delta t \)) of elementary processes, and a large one \( t \equiv N\Delta t \), which describes the time of evolution of the system. The ratio of these two time scales is assumed to be a very large number \( N \), so that the evolution in time can in fact be described by differential equations, leading to exponential behaviors with respect to time \( \sim \exp(\kappa t/\Delta t) \). The second criterion does not depend on any time scale and involves numbers only, as the generation number \( I \). In fact, the latter does not need to be very large. This property is important for practical purposes, as the second criterion describes the evolution of the system with respect to its energy content and is more pertinent for determining the criticality of the system, for example in nuclear reactors.

In the second criterion, the number \( N \) corresponds to an upper bound in the partial resummation over all time steps. The very large but finite value of \( N \equiv t/\Delta t \) gives an approximation to the infinite sum. The latter is controled by the ratio between the overall evolution time \( t \) of the system and the infinitesimal time step \( \Delta t \). The finite \( N \) approximation then does not play a role in establishing the asymptotic regime for the second criterion but may affect the eigenvalue which determines the critical behavior of generations. The precise
relation between the two criteria is studied in next sections.

C. Comparison of criticality criteria

First, the following property is easily proven:

(i) if \( \lambda_S < 1 \), then \( \lambda_T < 1 \)

(ii) if \( \lambda_T \geq 1 \), then \( \lambda_S \geq 1 \)

This property is a consequence of the following relations implied by the definitions of the mean particle and generation numbers and by their asymptotic behaviors (26)

\[
\sum_{I,\alpha} n_I(\alpha) \leq \sum_{N,\alpha} \bar{n}_\alpha(N\Delta t) \leq \sum_{N,\alpha} \bar{n}_\alpha(N\Delta t) < \infty \iff \lambda_S < 1 \quad \text{(27)}
\]

In fact, one can prove a more refined result:

(i) \( \lambda_T = 1 \) if and only if \( \lambda_S = 1 \)

(ii) \( \lambda_T < 1 \) if and only if \( \lambda_S < 1 \), in which case \( \lambda_T \leq \lambda_S < 1 \)

(iii) \( \lambda_T > 1 \) if and only if \( \lambda_S > 1 \), in which case \( 1 < \lambda_S \leq \lambda_T \)

Property (i) is a direct consequence of relation (24) between matrices \( S \) and \( T \), recalling that \( 1 - R \) is invertible. We now prove properties (ii) and (iii).

We define \( w \equiv (1 - R)^{-1}v^0(T) \), so that

\[
Fw = T v^0(T) = \lambda_T(1 - R)w
\]

\[
Sw = Rw + Fw = \lambda_T w + (1 - \lambda_T)Rw
\]  

(28)

Noting that \( 1 - R, v^0(T) \), hence \( w \), and \( R \), hence \( Rw \), have only positive elements, one first deduces that

\[
\lambda_T \leq 1 \quad \Rightarrow \quad (Sw)_\alpha \geq \lambda_Tw_\alpha
\]

\[
\Rightarrow \quad \lambda_S = \max_{v^0 > 0} \min_\alpha \left( \frac{(Sv)_\alpha}{v_\alpha} \right) \geq \min_\alpha \frac{(Sw)_\alpha}{w_\alpha} \geq \lambda_T
\]  

(29)

On the other hand, defining \( z \equiv (1 - R)^{-1}v^0(S) \), one has

\[
Tz = Fv^0(S) = \lambda_S(1 - R)^{-1}z - R(1 - R)^{-1}z
\]

\[
= (\lambda_S - 1)(1 - R)^{-1}z + z
\]  

(30)
Then, noting that $v^0$, $z$ and $R^n$ have only positive elements, so that $((1 - R)^{-1}z)_\alpha \geq z_\alpha$, one also deduces that

$$\lambda_S \geq 1 \quad \Rightarrow \quad \frac{(Tz)_\alpha}{z_\alpha} \geq \lambda_S$$

$$\Rightarrow \quad \lambda_T = \max_{v > 0} \min_\alpha \left( \frac{(Tv)_\alpha}{v_\alpha} \right) \geq \min_\alpha \left( \frac{(Tz)_\alpha}{z_\alpha} \right) \geq \lambda_S \quad (31)$$

Equations (29) and (31) may be summarized as

$$\lambda_T < 1 \quad \Rightarrow \quad \lambda_T \leq \lambda_S < 1$$

$$\lambda_S > 1 \quad \Rightarrow \quad \lambda_T \geq \lambda_S > 1 \quad (32)$$

Then, one knows that for any matrix $M$, $(1 - xM)^{-1} \equiv \sum_{n=0}^{\infty} x^n M^n$ is a convergent series provided that $|x| < 1 / \max(\text{Spec}(M))$. If $M$ is a matrix with positive elements, the radius of convergence is given by $1 / \lambda_M$. Now, assuming $\lambda_S \leq 1$ and noting that $R$ and $T$ have only positive elements, one has

$$(1 - xS)^{-1} = (1 - R)^{-1} (1 - (x - 1)R(1 - R)^{-1} - xF(1 - R)^{-1})^{-1}$$

$$\lambda_S < 1 \quad \Rightarrow \quad \sum_{n=0}^{\infty} \left( (x - 1)R(1 - R)^{-1} + xT \right)^n < \infty, \quad \forall x : 1 \leq |x| < \frac{1}{\lambda_S}$$

$$\Rightarrow \quad \sum_{n=0}^{\infty} (xT)^n < \infty, \quad \forall x : 0 \leq |x| < \frac{1}{\lambda_S}$$

$$\Rightarrow \quad \frac{1}{\lambda_S} \leq \frac{1}{\lambda_T} \quad (33)$$

Inequalities (32) and (33) provide parts (ii) and (iii) of the result.

### D. Perturbation around criticality

We consider now a system which depends on an additional parameter $s$, so that it is described by $s$-dependent matrices $(R(s), F(s))$ and $(S(s), T(s))$, and which remains near criticality ($\lambda_S(0) = \lambda_T(0) = 1$ for $s = 0$). We show that, in the neighborhood of criticality, a simple relation exists between the eigenvalues of the two matrices $S(s)$ and $T(s)$

$$\lambda_T(s) - 1 = r(\lambda_S(s) - 1), \quad r > 1 \quad (34)$$

As a consequence of the theorem of previous section, the proportionality coefficient $r$ must be greater than 1. We shall determine its value and show that it only depends on the matrix $R$ and on the eigenvectors of $S$ and $T$ evaluated at criticality.
To simplify the notations we shall write \( u^0(S(s)) \equiv u(s), u^0(T(s)) \equiv \tilde{u}(s) \) and \( v^0(S(s)) \equiv v(s), v^0(T(s)) \equiv \tilde{v}(s) \)

\[
\begin{align*}
u(s)S(s) &= \lambda_S(s)u(s), \quad S(s)v(s) = \lambda_S(s)v(s) \\
\tilde{u}(s)T(s) &= \lambda_T(s)\tilde{u}(s), \quad T(s)\tilde{v}(s) = \lambda_T(s)\tilde{v}(s)
\end{align*}
\] (35)

One also has from equation (24)

\[
(1 - S(s)) = (1 - T(s))(1 - R(s))
\]

\[
\Rightarrow \quad u(0) = \tilde{u}(0) \\
v(0) = (1 - R(0))^{-1}\tilde{v}(0)
\] (36)

Assuming differentiability in the parameter \( s \), we obtain from equations (35) (eigenvectors are normalized)

\[
\begin{align*}
\frac{d\lambda_S(s)}{ds} \bigg|_{s=0} &= \left( u(0)\frac{dS}{ds} \bigg|_{s=0} \right) \frac{1}{u(0)v(0)} \\
\frac{d\lambda_T(s)}{ds} \bigg|_{s=0} &= \left( \tilde{u}(0)\frac{dT}{ds} \bigg|_{s=0} \right) \frac{1}{\tilde{u}(0)\tilde{v}(0)}
\end{align*}
\] (37)

One deduces from (36)

\[
\begin{align*}
\frac{dT}{ds} &= \left( \frac{dS}{ds} + (T - 1)\frac{dR}{ds} \right) (1 - R)^{-1} \\
\Rightarrow \quad \tilde{u}(0)\frac{dT}{ds} \bigg|_{s=0} = u(0)\frac{dS}{ds} \bigg|_{s=0} v(0)
\end{align*}
\] (38)

From equations (37) and (38), one deduces the following relation between the variations of the two eigenvalues determining criticality

\[
\frac{d\lambda_T(s)}{ds} \bigg|_{s=0} = \frac{d\lambda_S(s)}{ds} \bigg|_{s=0} \frac{u(0)v(0)}{u(0)(1 - R(0))v(0)}
\] (39)

Relation (34) is thus deduced in the vicinity of criticality, with the following value for the proportionality coefficient

\[
r = \frac{u(0)v(0)}{u(0)(1 - R(0))v(0)} = \sum_n \left( \frac{u(0)R(0)^n v(0)}{u(0)v(0)} \right)^n
\]

\[
u(0) : \quad u(0) = u(0)S(0) = u(0)T(0) \\
v(0) : \quad v(0) = S(0)v(0) = (1 - R(0))^{-1}T(0)(1 - R(0))v(0)
\] (40)

The proportionality coefficient \( r \) is in effect greater than 1. Moreover, the general properties of the two eigenvalues characterizing criticality, which have been briefly stated in a previous
section, may now be discussed explicitly. One sees from equation (40) that the ratio $r$ of their distances to 1 is indeed proportional to $\frac{\tau}{\Delta t}$, where $\tau \equiv \frac{1}{\dot{R}(0)}$ is a characteristic time for evolution, without fission, of the system at criticality. The ratio $r$ may be seen as the mean number of time steps occurring during an elementary propagation process (without fission), or else as the inverse of the probability of propagation without fission. Equations (34) and (40) show that when this probability decreases, then the distance to criticality increases. Also, the second criterion appears to be more efficient than the first one when determining the distance to criticality.

V. CONCLUSION

In this article, using a suitable formalism, we have described the evolution of a nuclear reactor core both in terms of neutron generations and in time. These two descriptions have led to two corresponding estimates of the multiplication factor, hence to two different criteria for criticality. These two estimates have nonetheless been shown to be tightly related, one being bounded by the other near criticality. This result confirms the intuitive picture, that both definitions of criticality should be equivalent, namely that the number of neutrons should increase exponentially in time if and only if it does so in terms of generations. More precisely, we have obtained a rigorous comparison of the multiplication factors defined as the largest eigenvalues of the matrices describing the evolution of neutron fluxes, both with criticality and with respect to each other.

This result provides the justification for extending the application of the generation approach to Monte Carlo simulations to ADS and for using the deduced global parameters characterizing the system for a comparison with criticality. Amplification power and efficiency of the whole system can thus be directly and simply connected with a $k_{\text{eff}}$ coefficient which can be computed using the generation approach. This gives confidence in the ability to use global criteria for maintaining a secure evolution of subcritical systems [18, 19] and strengthens the argument in favor of the safeness capabilities of ADS designs.

Moreover, the formalism used here allows one to simultaneously follow the evolution of a nuclear core in the generation and the time dependent approaches. This allows one to connect the parameters which characterize the global state of a nuclear core in a time
independent way to the time dependent properties of neutron fluxes. This should help one to fill the gap usually separating the values for global parameters which are obtained from simulations and those which are deduced from direct measurements, in the case of heterogeneous systems such as ADS \cite{10, 12}. This should help to significantly improve the comparison between modelizations and experimental realizations of ADS, and hence to simulate and test realistic design in a way which remains close to practical setups and to technical requirements.

Let us finally remark that applications of the present study are not limited to the case of the multiplicative processes determining the evolution of nuclear reactor cores. Multiplicative processes also often appear in various chemical or biological reaction chains, for instance in molecular biology, genetics or population evolutions. Due to their multiplicative character, the processes underlying these systems lead to equations describing their time evolution which are similar to those governing neutron fluxes in a nuclear reactor core. The formalism developed here could show helpful for their modelization and lead to new hindsights for their understanding.

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