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Notes on the Lumped Backward Master Equation for the Neutron Extinction/Survival Probability

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1 Introduction

The expected or mean neutron number (or density) provides an adequate characterization of the neutron population and its dynamical excursions in most neutronic applications, in particular power reactors. Fluctuations in the neutron number, originating from the inherent randomness of neutron interactions and fission neutron multiplicities, are relatively small and ignorable for operational purposes, although measurements of the variance and time correlations provide valuable diagnostic information on fundamental reactor physics parameters. However, it is well known [1] that there exist situations of great interest and importance in which a strictly deterministic description, or even one supplemented with a knowledge of low order statistical averages (variance, correlation), provides an incomplete and very unsatisfactory description of the state of the neutron population. These situations are marked by persistent large fluctuations in the neutron number where the emergence of a deterministic phase is suppressed. Such situations are strongly stochastic and therefore unpredictable (i.e., the mean is not representative of the actual population), and can arise either by design or by accident. Examples where the stochastic behavior of neutron populations must be taken into account include: nuclear weapon single-point safety assessment; criticality excursions in spent fuel storage and in the handling of fissile solutions in fuel fabrication and reprocessing; approach to critical under suboptimal reactor start-up conditions; preinitiation in fast burst research reactors; and weak nuclear signatures in the passive detection of nuclear materials.

What distinguishes strongly stochastic neutronic systems from strongly deterministic systems is that, in the former, neutron multiplication occurs in the presence of weak neutron sources, such as spontaneous fission and background (cosmic) radiation. Weak sources (in a sense that can be made quite precise) lead to well separated fission chains (a fission chain is defined as the initial source neutron and all its subsequent progeny) in which some chains are short lived while others propagate for unusually long times. Under these conditions, fission chains do not overlap strongly and this precludes the cancellation of neutron number fluctuations necessary for the mean to become established as the dominant measure of the neutron population. The fate of individual chains then plays a defining role in the evolution of the neutron population in strongly stochastic systems, and of particular interest and importance in supercritical systems is the *extinction probability*, defined as the probability that the neutron chain (initiating neutron and its progeny) will be extinguished at a particular time, or its complement, the time-dependent *survival probability*. The time-asymptotic limit of the latter, the *probability of divergence*, gives the probability that the neutron population will grow without bound, and is more commonly known as the *probability of initiation* or just POI. The ability to numerically compute these probabilities, with high accuracy and without overly restricting the underlying physics (e.g., fission neutron multiplicity, reactivity variation) is clearly essential in developing an understanding of the behavior of strongly stochastic systems.

The theory of continuous time Markov processes [2, 3, 4, 5, 6] provides a general probabilisitic framework for the description of stochastic neutron populations. For point or lumped systems, differential Chapmann-Kolmogorov or so-called Master equations of the forward and backward type can be derived for the probability of finding a certain number of neutrons as a function of time [7, 5, 13, 6, 8, 9]. Both approaches yield systems of differential-difference equations for the neutron number probability distribution function (pdf), with the distinction that the backward Master equation is nonlinear in the pdf while the forward equation is linear. Another difference is that while any intrinsic or external source can be included explicitly in the forward Master equation, the backward approach describes the fate of a single neutron chain and must be supplemented with an auxiliary equation to account for a random neutron source. Thus, although the information content of these equations is formally the same, namely the neutron number distribution, the solution of each equation presents different challenges. This is particularly true for the computation of the chain survival and divergence probabilities of interest here and as discussed below. For nonlumped systems, where the neutron phase-space cannot be ignored, the backward formulation is the only viable approach for the computation of the survival and divergence probabilities [12, 13, 14, 15, 16] but it is computationally expensive in multidimensional, energy dependent applications. A point or lumped model, on the other hand, that incorporates leakage effects through an effective multiplication factor provides an efficient method of generating quantitative results and is particularly useful in conducting comprehensive parametric investigations.

The forward approach [7, 5, 6, 8, 9] requires the complete neutron number distribution function to be first obtained from which the extinction/survival probability is extracted as a special case [7, 8, 9]. However, since the equations for the number distribution are not closed, direct numerical solution requires this set to be truncated at a suitable order which, however, may be too high for this approach to be computationally practical. For instance, in the estimation of the divergence probability it is necessary to consider neutron numbers typically in the millions in order for a chain to potentially be declared as diverged. Even for a lumped model, numerical solution of such large systems of equations is impractical. Moreover, given the nonzero (albeit small) probability of extinction of even a large population, in practice the exact or theoretical POI cannot be computed without an irreducible error using the forward approach. Monte Carlo simulation of chain growth is subject to a similar constraint on the chain length that can realistically be managed, and the simulation must be terminated either after a fixed time or when the chain has reached a prescribed length (however, see Booth [10] for a recently proposed variance reduction scheme). Closed form analytic solutions for the neutron number distribution after transforming to the generating function formulation, on the other hand, are only possible when significant simplifications of the underlying physical models are introduced, in particular for the fission neutron multiplicity. The quadratic approximation introduced by Bell [7, 6, 8, 9] enables an exact solution of the forward Master equation to be obtained but yields accurate results only for weakly supercritical systems and large neutron populations. Singlet-emitting steady sources and a static-alpha are additional constraints typically necessary in order to obtain closed form solutions for the number distribution in the presence of an intrinsic source. Under less restrictive constraints on the physical models and parameters - when the system reactivity, and potentially the source strength, are arbitrary functions of time and when it is essential to use a general model of fission neutron multiplicity (both for the source and induced fission), and not some convenient approximation - the forward Master equation is intractable to general solution.

The backward approach, as will be developed below, yields a closed form nonlinear differential equation directly for the time dependent survival probability for a single neutron chain under general conditions, thereby bypassing the need to first solve the hierarchy of differential-difference equations for the number distribution. An auxiliary differential equation then relates the survival probability when a random intrinsic (spontaneous fission) source of arbitrary multiplicity is present to that for a single neutron chain. Both equations can be easily solved without further approximation using standard numerical methods for first order nonlinear ordinary differential equations, which greatly expands the scope of relevancy of the results and makes it possible to quantitatively assess the accuracy of various approximations employed in the forward formulation. Moreover, the explicit form of the equations enables the effect of uncertainty in the fundamental parameters (multiplicities, lifetime, alpha) on the survival probability and the POI to be accurately evaluated.

The purpose of these notes is to present a detailed derivation of the backward Master equation for the chain survival probability in a lumped-model setting. The relevant equation can, of course, be extracted from Bell's general equation for an unlumped system [12] by striking the streaming term and eliminating the energy and direction dependence. It is, however, instructive to derive the lumped model equation from first principles and directly in differential form [13] as opposed to the integral form that results from the traditional derivation based on the regeneration point technique [12, 6]. The possibilities arising from a relatively small investment in numerical effort become clear while limitations are also apparent. It is hoped that the pedagogical development of the lumped backward Master equation formulation as encapsulated in these notes will prove of some value to the nonexpert and expert reader alike.

The scope of these notes is as follows. The hierarchy of backward equations for the neutron number probability distribution function for a single chain is derived directly in differential form, using probability balance arguments familiar from continuous time Markov process theory, and transformed to a single nonlinear partial differential equation for the generating function. Noting a special property of the backward formulation, the generating function equation is then reduced to the desired nonlinear ordinary differential equation for the time-dependent survival probability. Next, an auxiliary equation is obtained that relates the survival probability for neutron chains initiated by a random source of arbitrary multiplicity to the extinction (or survival) probability for a single neutron chain. A closed form analytic solution is then obtained in the quadratic approximation and shown to be equivalent of that obtained previously using the forward Master equation with and without the random source. Finally, we make some remarks on the numerical solution of the survival probability equation for a single chain as well as for chains initiated by a random source of neutrons.

2 Backward Master Equation

We begin with some definitions. Let τ be the neutron lifetime. The probability that a neutron experiences an interaction in a short time Δs is then given by $\Delta s/\tau$, which follows from the Markovian property of neutron interactions. Let p_f be the probability that the interaction is fission and let p_ν be the fission neutron multiplicity, i.e., probability that ν prompt neutrons $(\nu = 0, 1, \ldots \nu_{max})$ are emitted in a fission. The multiplicity distribution is assumed to be normalized:

$$\sum_{\nu=0}^{\nu_{max}} p_\nu = 1, \tag{1}$$

so that the mean number of fission neutrons is given by:

$$\overline{\nu} = \sum_{\nu=0}^{\nu_{max}} \nu\, p_\nu, \tag{2}$$

and the factorial moments are defined as:

$$\chi_m = \sum_{\nu=0}^{\nu_{max}} \nu(\nu-1)\cdots(\nu-m+1)\, p_\nu, \quad m = 1, 2, \ldots \nu_{max}\,. \tag{3}$$

Similarly, we define the source factorial moments as:

$$\chi_m^s = \sum_{k=0}^{K_s} k(k-1)\cdots(k-m+1)\, q_k, \quad m = 1, 2, \ldots K_s\,. \tag{4}$$

The physical interpretation of the factorial moments is that $\chi_2/2!$ is the mean number of neutron doublets, $\chi_3/3!$ is the mean number of neutron triplets, $\cdots$ $\chi_m/m!$ the mean number of neutron m-tuplets, from a single fission. The probability that a neutron interaction results in the production of j prompt neutrons is then expressed as $p_f\, p_j\, \Delta s/\tau = c_j\, \Delta s/\tau$, $j = 0, 1, \ldots \nu_{max}$. We also define $\overline{c}_0 = 1 - p_f$ as the probability of all non-fission events, such as parasitic capture and leakage, in which case the interacting neutron is considered lost from the system. Finally, the probability that a source decays in Δs is $\mathcal{S}\Delta s$ and the probability that the decay results in k prompt neutrons is q_k, $k = 0, 1, \ldots K_s$, which again is normalized as $\sum_{k=0}^{K_s} q_k = 1$. The quantity:

$$\overline{S} = \mathcal{S} \sum_{k=0}^{K_s} k\, q_k = \mathcal{S}\, \overline{k} \tag{5}$$

is the mean rate of generation of source neutrons, or the source strength. Thus, for a singlet emitting source, $q_k = \delta_{k,1}$ and the source strength is just $\mathcal{S}$. Note that by "source neutrons" we refer to neutrons appearing in the system through a mechanism that is independent of the instantaneous neutron population. Such sources are often referred to as "fixed", "volume" or "external" sources to distinguish them from neutrons produced in fission reactions (or through other nuclear processes) that are induced by existing neutrons. Examples of neutron sources include spontaneous fission, spallation reactions, background (cosmic) neutrons, $(n, 2n)$ reactions, amongst many others.

We now perform a balance of all independent and mutually exclusive elementary events to develop an equation for the probability $P_n(t|s)$, $n \geq 0$, of finding precisely n neutrons in the system at time t given one neutron introduced into the system at s. $P_n(t|s)$ is defined to be zero for $t < s$ and $n < 0$. The balance in the backward approach is done in the first collision interval so that the operational time is the initial time variable s, in contrast to the forward approach where the balance is done over the last collision interval and the final time is then the variable time. Specifically, we consider the transitions that the initial neutron can undergo in the short time between s and Δs and use the Markov property to account for all subsequent transitions, over the time interval $(s + \Delta s, t)$, that contribute to the final state. We note that it is not possible in the backward approach to write down a closed equation for the survival probability when the medium contains an intrinsic random source. In this case, as will be shown below, the survival probability must be obtained through an auxiliary equation that explicitly depends on the survival probability of a single chain.

The probability balance can be stated as:

$$\begin{aligned} P_n(t|s) = (1 - \frac{\Delta s}{\tau})P_n(t|s + \Delta s) + \bar{c}_0\frac{\Delta s}{\tau}\delta_{n,0} + \Bigg\{ c_0\frac{\Delta s}{\tau}\delta_{n,0} + c_1\frac{\Delta s}{\tau}P_n(t|s + \Delta s) + \\ + c_2\frac{\Delta s}{\tau}\sum_{n_1+n_2=n} P_{n_1}(t|s + \Delta s)P_{n_2}(t|s + \Delta s) + \\ + c_3\frac{\Delta s}{\tau}\sum_{n_1+n_2+n_3=n} P_{n_1}(t|s + \Delta s)P_{n_2}(t|s + \Delta s)P_{n_3}(t|s + \Delta s) + \ldots \Bigg\} \end{aligned} \tag{6}$$

In Eq.(6), the various terms on the right hand side have the following physical interpretations:

- The first term expresses the probability that there is no interaction in Δs and the neutron does not leak from the system, and, for this event to contribute to the final state, the probability must be multiplied by the probability that n neutrons will be produced by this neutron over the subsequent time interval $(s + \Delta s, t)$.
- The second term expresses the probability that the neutron is radiatively captured or leaks from the system, and this event will contribute to the final state only if the final state is empty, i.e, $n = 0$.
- The remaining terms, those in braces, account for the contribution to the final state from fission neutrons of various multiplicities. Thus:
  - the first term expresses the probability that 0 neutrons are produced in fission, and this event will contribute to the final state only if the final state is empty, i.e, $n = 0$,

– the second term expresses the probability that 1 neutron is produced in fission, and this probability must be multiplied by the probability that the fission neutron will lead to n neutrons over the subsequent time interval $(s + \Delta s, t)$,

– the third term expresses the probability that 2 neutrons are produced in fission, and this probability must be multiplied by the probability that both these neutrons will *independently* and *collectively* result in exactly n neutrons over the subsequent time interval $(s + \Delta s, t)$,

– the third term expresses the probability that 3 neutrons are produced in fission, and this probability must be multiplied by the probability that these 3 neutrons will *independently* and *collectively* result in exactly n neutrons over the subsequent time interval $(s + \Delta s, t)$,

– the terms corresponding to higher numbers of fission neutrons have similar interpretations.

By rearranging terms, Eq.(6) can be conveniently expressed as:

$$\begin{aligned}\frac{P_n(t|s) - P_n(t|s+\Delta s)}{\Delta s} &= -\frac{1}{\tau}P_n(t|s+\Delta s) + \overline{c}_0\frac{1}{\tau}\delta_{n,0} + \left\{ c_0\frac{\Delta s}{\tau}\delta_{n,0} + \frac{1}{\tau}c_1 P_n(t|s+\Delta s) + \right. \\ &+ \frac{1}{\tau}\sum_{n_1+n_2=n} c_2 P_{n_1}(t|s+\Delta s)P_{n_2}(t|s+\Delta s) + \\ &\left. + \frac{1}{\tau}\sum_{n_1+n_2+n_3=n} c_3 P_{n_1}(t|s+\Delta s)P_{n_2}(t|s+\Delta s)P_{n_3}(t|s+\Delta s) + \ldots \right\}.\end{aligned} \tag{7}$$

Taking the limit $\Delta s \to 0$ transforms Eq.(7) into the differential equation:

$$\begin{aligned}-\frac{\partial P_n(t|s)}{\partial s} &= -\frac{1}{\tau}P_n(t|s) + \overline{c}_0\frac{1}{\tau}\delta_{n,0} + \left\{ c_0\frac{1}{\tau}\delta_{n,0} + \frac{1}{\tau}c_1 P_n(t|s) + \right. \\ &+ \frac{1}{\tau}\sum_{n_1+n_2=n} c_2 P_{n_1}(t|s)P_{n_2}(t|s) + \\ &\left. + \frac{1}{\tau}\sum_{n_1+n_2+n_3=n} c_3 P_{n_1}(t|s)P_{n_2}(t|s+\Delta s)P_{n_3}(t|s) + \ldots \right\},\end{aligned} \tag{8}$$

or, more compactly,

$$-\frac{\partial P_n(t|s)}{\partial s} = -\frac{1}{\tau}P_n(t|s) + \bar{c}_0\frac{1}{\tau}\delta_{n,0} + \frac{1}{\tau}\sum_{k=0}^{\nu_{max}} \sum_{n_1+n_2+\cdots n_k=n} c_k \prod_{j=1}^{k} P_{n_j}(t|s), \quad s \le t, \tag{9a}$$

where the c_0 term corresponding to zero fission neutrons has been incorporated into the summation and it is understood that the product is unity when $k = 0$. The solution to this equation is subject to the "final time" condition:

$$\lim_{s\to t} P_n(t|s) = \delta_{n,1}. \tag{9b}$$

That is, when the initial time of neutron injection corresponds to the final time t, the probability of finding any number of neutrons is zero unless $n = 1$ in which case it is a certainty.

Eq.(9a) is the backward differential Chapmann-Kolmogorov equation, also known as the backward Master equation, for the neutron number probability distribution function. It is a nonlinear differential equation, with nonlinearity of degree ν_{max}, and must be solved in reverse time. That is, given the final condition Eq.(9b) at some fixed time t, the solution proceeds backwards to some earlier time s where $-\infty < s \le t$. Although the backward equation differs markedly in mathematical structure from the linear forward equation, they are both valid formulations of the neutron number distribution function $P_n(t|s)$. It is often remarked that the choice between forward or backward formulations is a matter of taste, but in many situations one approach may have distinct advantages over the other, as will be illustrated in these notes.

3 Equation for the Generating Function

The set of nonlinear differential-difference equations given by Eq.(9a) can be converted into a nonlinear partial differential equation for the generating function from which an equation for the survival probability can be derived. The ordinary generating function is defined by the discrete transformation:

$$G(x, s) = \sum_{n=0}^{\infty} x^n \, P_n(t|s), \quad s \le t, \tag{10}$$

where x is a real, continuous variable and the final time t has been suppressed as an argument of G for notational convenience. Since the P_n are normalized, i.e., $\sum_{n=0}^{\infty} P_n = 1$, it follows that the sum in Eq.(10) converges for $0 \le x \le 1$ (we note, however, that the radius of convergence of this sum may exceed unity). Applying this transform successively to each term in Eq.(9a), we note that the left hand side and the first two terms on the right hand side transform trivially but the terms involving the multiplicities are more complex. Consider the transform of the term corresponding to multiplicity order k:

$$
\begin{aligned}
I_k(x,s) &= \sum_{n=0}^{\infty} x^n \sum_{n_1+n_2+\cdots n_k=n} \prod_{j=1}^{k} P_{n_j}(t|s), \\
&= \sum_{n=0}^{\infty} x^n \sum_{n_1=0}^{\infty} P_{n_1} \sum_{n_2=0}^{\infty} P_{n_2} \cdots \sum_{n_k=0}^{\infty} P_{n_k}, \quad n_1+n_2+\cdots n_k = n, \\
&= \sum_{n_1=0}^{\infty} P_{n_1} \sum_{n_2=0}^{\infty} P_{n_2} \cdots \sum_{n_{k-1}=0}^{\infty} P_{n_{k-1}} \sum_{n=0}^{\infty} x^n P_{n-(n_1+n_2+\cdots n_{k-1})}
\end{aligned}
\tag{11}
$$

Setting $m = n - (n_1 + n_2 + \cdots n_{k-1})$ in Eq.(11) and rearranging terms gives:

$$
\begin{aligned}
I_k(x,s) &= \sum_{n_1=0}^{\infty} x^{n_1} P_{n_1} \sum_{n_2=0}^{\infty} x^{n_2} P_{n_2} \cdots \sum_{n_{k-1}=0}^{\infty} x^{n_{k-1}} P_{n_{k-1}} \sum_{m=-(n_1+n_2+\cdots n_{k-1})}^{\infty} x^m P_m, \\
&= \sum_{n_1=0}^{\infty} x^{n_1} P_{n_1} \sum_{n_2=0}^{\infty} x^{n_2} P_{n_2} \cdots \sum_{n_{k-1}=0}^{\infty} x^{n_{k-1}} P_{n_{k-1}} \sum_{m=0}^{\infty} x^m P_m, \\
&= [G(x,s)]^k,
\end{aligned}
\tag{12}
$$

where, in going from the first to the second line, we have noted that $P_m = 0$ for $m < 0$, by definition. The equation for the generating function finally becomes:

$$
-\frac{\partial G(x,s)}{\partial s} = \frac{\overline{c}_0}{\tau} - \frac{1}{\tau} G(x,s) + \frac{1}{\tau} \sum_{k=0}^{\nu_{max}} c_k \, [G(x,s)]^k \tag{13a}
$$

$$
\lim_{s \to t} G(x,s) = x. \tag{13b}
$$

We note that if the generating function for the neutron multiplicity is defined as:

$$
g(x) = \sum_{k=0}^{\nu_{max}} x^k \, p_k,
$$

then, upon substituting $c_k = p_f \, p_k$ in Eq.(13a), the equation for G can be written compactly as:

$$
-\frac{\partial G(x,s)}{\partial s} = \frac{\overline{c}_0}{\tau} - \frac{1}{\tau} G(x,s) + \frac{p_f}{\tau} g(G)
$$

For purposes of obtaining an equation for the survival probability, it is expedient to express the above equation in terms of the variable $\widetilde{G}$ defined by [12]:

$$\widetilde{G}(x,s) = 1 - G(x,s). \tag{14}$$

Substituting for G from Eq.(14) into Eqs.(13a) & (13b) and using a binomial expansion to expand the nonlinear terms, we obtain:

$$\begin{aligned}\frac{\partial \widetilde{G}(x,s)}{\partial s} &= \frac{\bar{c}_0}{\tau} - \frac{1}{\tau}\left[1-\widetilde{G}(x,s)\right] + \frac{1}{\tau}\sum_{k=0}^{\nu_{max}} c_k \left[1-\widetilde{G}(x,s)\right]^k, \\ &= \frac{\bar{c}_0}{\tau} - \frac{1}{\tau}\left[1-\widetilde{G}(x,s)\right] + \frac{1}{\tau}\sum_{k=0}^{\nu_{max}} c_k \sum_{i=0}^{k} (-1)^i \frac{k!}{(k-i)!i!}\, \widetilde{G}^i(x,s) \end{aligned} \tag{15}$$

The last term on the right hand side of the above equation can be further simplified to give:

$$\begin{aligned}\frac{1}{\tau}\sum_{k=0}^{\nu_{max}} c_k \sum_{i=0}^{k} (-1)^i \frac{k!}{(k-i)!i!}\, \widetilde{G}^i(x,s) &= \frac{1}{\tau}\sum_{i=0}^{\nu_{max}} \frac{(-1)^i}{i!} \widetilde{G}^i(x,s) \sum_{k=i}^{\nu_{max}} \frac{k!}{(k-i)!}\, c_k, \\ &= \frac{p_f}{\tau}\sum_{i=0}^{\nu_{max}} (-1)^i\, \frac{\chi_i}{i!}\, \widetilde{G}^i(x,s), \end{aligned} \tag{16}$$

where we have introduced the factorial moments χ_i defined in Eq.(3). Inserting the above result into Eq.(15) finally yields:

$$\frac{\partial \widetilde{G}(x,s)}{\partial s} = \frac{\bar{c}_0}{\tau} - \frac{1}{\tau}\left[1-\widetilde{G}(x,s)\right] + \frac{p_f}{\tau}\sum_{k=0}^{\nu_{max}} (-1)^k\, \frac{\chi_k}{k!}\, \widetilde{G}^k(x,s), \tag{17a}$$

with final condition:

$$\lim_{s\to t} \widetilde{G}(x,s) = 1 - x. \tag{17b}$$

4 Single Chain Extinction/Survival Probability

The quantity $P_0(t|s)$ is known as the extinction probability, and is defined as the probability that, given one neutron in the medium at time s, the neutron population will vanish at some later time t. It then follows that:

$$\begin{aligned}1 - P_0(t|s) &= \sum_{n=0}^{\infty} P_n(t|s) - P_0(t|s), \\ &= \sum_{n=1}^{\infty} P_n(t|s), \\ &= P(t|s), \end{aligned} \tag{18}$$

which defines the survival or nonextinction probability. Further noting upon setting $x = 0$ in Eq.(10) that:

$$P_0(t|s) = G(0, s), \tag{19}$$

it follows from Eq.(14) that the survival probability can also be expressed in terms of the generating function:

$$P(t|s) = 1 - G(0, s) = \widetilde{G}(0, s). \tag{20}$$

Now observing that the variable x appears explicitly in the boundary condition, Eq.(17b), but only implicitly in the actual equation for the generating function, Eq.(17a), setting $x = 0$ trivially transforms the equation for $\widetilde{G}(x, s)$ into one for the survival probability, $P(t|s)$. Thus the survival probability satisfies the following nonlinear differential equation:

$$\frac{\partial P(t|s)}{\partial s} = \frac{\overline{c}_0}{\tau} - \frac{1}{\tau}\left[1 - P(t|s)\right] + \frac{p_f}{\tau}\sum_{k=0}^{\nu_{max}} (-1)^k \frac{\chi_k}{k!} P^k(t|s), \tag{21a}$$

with the appropriate final condition obtained by setting $x = 0$ in Eq.(17b):

$$\lim_{s \to t} P(t|s) = 1. \tag{21b}$$

Eq.(21a) can be simplified further by isolating the $k = 0$ term in the sum over the neutron multiplicity and rearranging to obtain:

$$\frac{\partial P(t|s)}{\partial s} = \frac{1}{\tau}\left[p_f - (1 - \overline{c}_0)\right] + \frac{1}{\tau}P(t|s) + \frac{p_f}{\tau}\sum_{k=1}^{\nu_{max}} (-1)^k \frac{\chi_k}{k!} P^k(t|s). \tag{22}$$

But recalling that $\overline{c}_0 = (1 - p_f)$, the first term on the right hand side of Eq.(22) vanishes to give:

$$\frac{\partial P(t|s)}{\partial s} = \frac{1}{\tau} P(t|s) + \frac{p_f}{\tau} \sum_{k=1}^{\nu_{max}} (-1)^k \, \frac{\chi_k}{k!} \, P^k(t|s), \tag{23}$$

or, also isolating the $k = 1$ term:

$$\frac{\partial P(t|s)}{\partial s} = -\frac{1}{\tau}(p_f \overline{\nu} - 1) P(t|s) + \frac{p_f}{\tau} \sum_{k=2}^{\nu_{max}} (-1)^k \, \frac{\chi_k}{k!} \, P^k(t|s). \tag{24}$$

Recognizing and introducing the multiplication factor k:

$$k = \overline{\nu} \, p_f, \tag{25}$$

and defining α as:

$$\alpha = \frac{k - 1}{\tau}, \tag{26}$$

we finally obtain the desired equation for the survival probability:

$$-\frac{\partial P(t|s)}{\partial s} = \alpha(s) P(t|s) - \frac{p_f(s)}{\tau} \sum_{k=2}^{\nu_{max}} (-1)^k \, \frac{\chi_k}{k!} \, P^k(t|s), \tag{27a}$$

with final condition:

$$\lim_{s \to t} P(t|s) = 1, \tag{27b}$$

where we have explicitly indicated that the fission probability and hence the multiplication factor can be a function of time. The negative sign on the time derivative underscores the fact that the backward equation describes a process that is adjoint in time. The mathematical problem is therefore well posed and, although we have not addressed existence and uniqueness of solutions to Eqs.(27a) – (27b), we note that a solution, if it exists and is unique, can be obtained by integrating backwards in time.

Finally, we remark that the probability of initiation (POI) is given by $\lim_{s \to -\infty} P(t|s)$, i.e., the initiating neutron is injected in the infinite past, and if a nonzero limit exists, the POI defines the probability that the neutron population will diverge [9]. Under these conditions, the POI is given by the nontrivial root that lies in the interval $(0, 1]$ of the nonlinear algebraic equation obtained by setting the time derivative in Eq.(27a) to zero:

$$\alpha(-\infty)POI - \frac{p_f(-\infty)}{\tau}\sum_{k=2}^{\nu_{max}}(-1)^k\,\frac{\chi_k}{k!}\,(POI)^k = 0. \tag{28}$$

It is readily shown that the only stable solution for the POI in subcritical and critical systems is zero while for supercritical systems a nonzero stable solution in the range $(0, 1]$ exists [4, 6]. For time varying α and p_f, the system criticality as determined by limiting values of these parameters as $t \to \infty$ (assumed bounded) dictates the possibility of divergence of the chain. We close this discussion by remarking that although the above equation based on the backward formulation allows the POI to be computed, to demonstrate that the POI corresponds to the probability that the neutron population has actually diverged requires a knowledge, and a careful limiting analysis, of the actual time dependent neutron number probability distribution [9].

5 Extinction/Survival Probability With Intrinsic Random Source

The backward Master equation cannot be generalized to account for the presence of an intrinsic random source as is readily done in the forward approach. The reason is quite simple: the operational variable in the backward approach is defined to be the time of injection of a source neutron and this definition loses uniqueness when source neutrons are repeatedly and randomly introduced into the system. To allow for a source, it is necessary to carry out a separate balance that accounts for random emission of source neutrons and their contribution to the neutron population at the final time.

Let $\Theta_n(t|t_0)$ be the probability that n neutrons will be found at time t given a neutron source that was “turned on” at some arbitrary time $t_0 \le t$. That is, there are no neutrons in the system prior to this time. Consider now the time interval $(t_0, t_0 + \Delta t_0)$ and events that are possible during Δt_0 that eventually lead to the final state. A probability balance can be written as follows:

$$
\begin{aligned}
\Theta_n(t|t_0) = {} & (1-\mathcal{S}\Delta t_0)\,\Theta_n(t|t_0+\Delta t_0)+ \\
& + \mathcal{S}\Delta t_0\, q_1 \sum_{n_1+m_1=n} P_{n_1}(t|t_0+\Delta t_0)\,\Theta_{m_1}(t|t_0+\Delta t_0)+ \\
& + \mathcal{S}\Delta t_0\, q_2 \sum_{n_1+n_2+m_2=n} P_{n_1}(t|t_0+\Delta t_0)\,P_{n_2}(t|t_0+\Delta t_0)\,\Theta_{m_2}(t|t_0+\Delta t_0)+ \\
& \vdots \\
& + \mathcal{S}\Delta t_0\, q_k \sum_{n_1+n_2+\cdots n_k+m_k=n} \prod_{j=1}^{k} P_{n_j}(t|t_0+\Delta t_0)\,\Theta_{m_k}(t|t_0+\Delta t_0)+ \\
& \vdots
\end{aligned}
\tag{29}
$$

In Eq.(29) the various terms on the right hand side have the following physical interpretations:

- The first term describes the event that no source neutron is emitted in Δt_0 and that the final state of n neutrons is attained by later source events in the interval $(t_0+\Delta t_0, t)$.
- The second term describes the event that 1 source neutron is emitted in Δt_0 which contributes n_1 neutrons to the final state with probability given by the single chain probability and with the difference $m_1 = n - n_1$ contributed by subsequent source events in the interval $(t_0+\Delta t_0, t)$.
- The third term describes the event that 2 source neutrons are emitted in Δt_0 which independently contribute n_1 and n_2 neutrons to the final state, with the difference $m_2 = n - n_1 - n_2$ contributed by subsequent source events in the interval $(t_0+\Delta t_0, t)$.
- The terms corresponding to higher numbers of source neutrons have similar interpretations.

Rearranging terms and taking the limit $\Delta t_0 \to 0$ yields the differential form:

$$
-\frac{\partial\Theta_n(t|t_0)}{\partial t_0} = -\mathcal{S}\Theta_n(t|t_0) + \mathcal{S}\sum_{k=1}^{K_s} q_k \sum_{n_1+n_2+\cdots n_k+m_k=n} \prod_{j=1}^{k} P_{n_j}(t|t_0)\,\Theta_{m_k}(t|t_0), \tag{30a}
$$

with the final condition:

$$
\lim_{t_0\to t}\Theta_n(t|t_0) = \delta_{n,0}. \tag{30b}
$$

This is consistent with the condition that no source neutrons can exist prior to the initial time which in this case is also the final time. We note that Eq.(30a) is linear in the probability Θ_n and depends on the neutron number probability corresponding to a single initial neutron which satisfies Eq.(9a). To solve Eq.(30a), we first transform it to an equation for the corresponding generating function which is defined as:

$$\mathcal{G}(x,t_0) = \sum_{k=0}^{\infty} x^k \Theta_n(t|t_0), \quad t_0 \leq t, \tag{31}$$

where the dependence of $\mathcal{G}$ on final time t is implicit. Using the same manipulations as before, it can be shown that this generating function satisfies:

$$-\frac{\partial \mathcal{G}(x,t_0)}{\partial t_0} = -\mathcal{S}\mathcal{G}(x,t_0) + \mathcal{S}\sum_{k=1}^{K_s} q_k \, [G(x,t_0)]^k \, \mathcal{G}(x,t_0), \tag{32a}$$

with the final condition:

$$\lim_{t_0 \to t} \mathcal{G}(x,t_0) = 1. \tag{32b}$$

Combining the two terms on the right hand side of Eq.(32a) yields the more compact form:

$$-\frac{\partial \mathcal{G}(x,t_0)}{\partial t_0} = \mathcal{S}\left[\sum_{k=1}^{K_s} q_k \, G^k(x,t_0) - 1\right] \mathcal{G}(x,t_0). \tag{33}$$

This is an elementary first order differential equation with a variable but known coefficient which can be solved by integrating backwards from the final condition Eq.(32b). The final result is:

$$\mathcal{G}(x,t_0) = \exp \int_{t_0}^{t} \mathcal{S}\left[\sum_{k=1}^{K_s} q_k \, G^k(x,t') - 1\right] dt', \quad t_0 \leq t, \tag{34}$$

From the definition in Eq.(31), $\mathcal{G}(0,t_0) = \Theta_0(t|t_0)$ is just the probability that the neutron population will become extinct at time t given that a random emitting source exists between (t_0,t). Thus, setting $x = 0$ and recalling that $G(0,t_0) = 1 - P(t|t_0)$, immediately transforms Eq.(33) to one for the extinction probability:

$$-\frac{\partial \Theta_0(t|t_0)}{\partial t_0} = \mathcal{S}\left[\sum_{k=1}^{K_s} q_k \, (1 - P(t|t_0))^k - 1\right] \Theta_0(t|t_0). \tag{35}$$

Expanding the integrand using the binomial theorem and introducing the source factorial moment notation further simplifies this result to:

$$-\frac{\partial \Theta_0(t|t_0)}{\partial t_0} = \mathcal{S}\left[\sum_{k=0}^{K_s} \frac{(-1)^k}{k!}\chi_k^s P^k(t|t_0) - 1\right] \Theta_0(t|t_0). \tag{36}$$

Finally, noting that $\chi_0^s = 1$, Eq.(36) reduces to the more convenient form:

$$-\frac{\partial \Theta_0(t|t_0)}{\partial t_0} = \mathcal{S}\left[\sum_{k=1}^{K_s} \frac{(-1)^k}{k!}\chi_k^s P^k(t|t_0)\right] \Theta_0(t|t_0), \tag{37a}$$

with the terminal condition:

$$\lim_{t_0 \to t} \Theta_0(t|t_0) = 1. \tag{37b}$$

Integrating Eqs.(37a) – (37b) gives for the extinction probability in the presence of a random source the explicit result:

$$\Theta_0(t|t_0) = \exp \int_{t_0}^{t} \mathcal{S}\left[\sum_{k=1}^{K_s} \frac{(-1)^k}{k!}\chi_k^s P^k(t|t_0)\right] dt'. \tag{38}$$

Thus, if the survival probability for a single chain is known, given by the solution of Eqs.(27a) – (27b), the above result gives the extinction probability for a neutron population that is driven by a random source of arbitrary multiplicity. The corresponding survival probability for the random source case is then simply obtained from:

$$\mathcal{P}_{\mathcal{S}}(t|t_0) = 1 - \mathcal{G}(0, t_0) = 1 - \Theta_0(t|t_0). \tag{39}$$

Note that the source-event probability $\mathcal{S}$ can in principle be time dependent and for this reason has been retained under the time integral in Eq.(38). For a singlet-emitting source, such that:

$$q_k = \delta_{k,1}, \quad \chi_k^s = \delta_{k,1}, \tag{40}$$

Eq.(38) reduces to a particularly simple and well known result:

$$\mathcal{P}_{\mathcal{S}}(t|t_0) = 1 - \exp\left[-\int_{t_0}^{t} \mathcal{S}\, P(t|t')dt'\right]. \tag{41}$$

This is just the classical formula of Bartlett [2, 6] and Eq.(38) provides the generalization of Bartlett's formula to multiplet-emitting sources.

6 Exact Solution in the Quadratic Approximation

To facilitate construction of closed form solutions to the forward Master equation, Bell [7, 8] introduced the quadratic approximation for a function that was closely related to the neutron multiplicity generating function. In addition to allowing an exact solution to be obtained for the neutron generating function and, by inversion of the generating function transform, the neutron number distribution function, the quadratic approximation has been shown to produce accurate neutron distributions for a marginally supercritical system at late times, i.e, when the mean number is large [7, 8]. In this section, we use the quadratic approximation to show that the nonlinear equation for the survival probability derived above can also be solved exactly for both single chain and random source scenarios and yields identical results to those obtained using the the forward approach.

The equivalent quadratic approximation in the backward formulation corresponds to truncating the nonlinear terms in the sum in Eq.(27a) at second order. The equation for the survival probability now reads:

$$-\frac{\partial P(t|s)}{\partial s} = \alpha(s)P(t|s) - \frac{p_f(s)\,\chi_2}{2\tau}\,P^2(t|s), \tag{42a}$$

with:

$$\lim_{s\to t} P(t|s) = 1. \tag{42b}$$

Eq.(42a) is a Bernoulli equation that can be solved by first transforming it to a linear differential equation using the variable change:

$$Q(t|s) = \frac{1}{P(t|s)}, \tag{43}$$

to get:

$$\frac{\partial Q(t|s)}{\partial s} = \alpha(s)Q(t|s) - \frac{p_f(s)\,\chi_2}{2\tau}, \tag{44a}$$

with:

$$\lim_{s\to t} Q(t|s) = 1. \tag{44b}$$

Eqs.(44a) & (44b) can be readily solved using the integrating factor technique, eventually obtaining for the survival probability:

$$P(t|s) = \frac{\exp\left[\int_s^t \alpha(s')ds'\right]}{1 + \frac{1}{2}\int_s^t ds'\, \chi_2'(s')\, \exp\left[\int_{s'}^t \alpha(s'')ds''\right]}, \quad s \leq t. \tag{45}$$

where we have defined:

$$\chi_2'(s) = \frac{p_f(s)\,\chi_2}{\tau}. \tag{46}$$

For a constant reactivity, so that α and χ_2' are independent of time, the integrals in Eq.(45) can be evaluated exactly and the result simplifies to:

$$P(t|s) = \frac{\exp \alpha(t-s)}{1 + \frac{1}{POI}\left[\exp \alpha(t-s) - 1\right]}, \quad s \leq t. \tag{47}$$

Here we have introduced the divergence probability or probability of initiation (POI) defined for static reactivity as [8]:

$$POI = \frac{2\alpha}{\chi_2'}. \tag{48}$$

The source survival probability follows upon inserting Eq.(45) for the single neutron survival probability into Eq.(41), but an explicit result can only be obtained for constant reactivity. Further assuming that the source emits only one neutron and substituting Eq.(47) into Eq.(41), the integral in the exponent can be evaluated as follows:

$$\begin{aligned}
\int_{t_0}^{t} \mathcal{S}\, P(t|t')dt' &= \mathcal{S} \int_0^{t-t_0} \frac{e^{\alpha u}}{1 + \frac{1}{POI}\left(e^{\alpha u} - 1\right)}\, du, \\
&= \mathcal{S}\, \frac{POI}{\alpha} \int_0^{t-t_0} \frac{\frac{\alpha}{POI} e^{\alpha u}}{1 + \frac{1}{POI}\left(e^{\alpha u} - 1\right)}\, du, \\
&= \mathcal{S}\, \frac{POI}{\alpha}\, \ln\left[1 + \frac{1}{POI}\left(e^{\alpha(t-t_0)} - 1\right)\right] \\
&= \ln\left[1 + \frac{1}{POI}\left(e^{\alpha(t-t_0)} - 1\right)\right]^{\eta},
\end{aligned} \tag{49}$$

where η is Bell's source parameter [7, 8] defined by:

$$\eta = \frac{2\mathcal{S}}{\chi_2'} = \mathcal{S}\,\frac{POI}{\alpha}. \tag{50}$$

Finally, inserting Eq.(49) into Eq.(41) gives for the source survival probability:

$$\mathcal{P}_{\mathcal{S}}(t|t_0) = 1 - \left[1 + \frac{1}{POI}\left(e^{\alpha(t-t_0)} - 1\right)\right]^{-\eta}. \tag{51}$$

Next, we demonstrate that Eqs.(45) & (51) for the survival probabilities are identical to those obtained using the forward Master equation.

6.1 Equivalence to Forward Master Equation Solution

In Ref. [8] the forward Master equation was exactly solved in the quadratic approximation to obtain the neutron number distribution function given one initial neutron, and the survival probability, obtained as the complement of the extinction probability, was shown to be:

$$P(t|s) = 1 - \frac{a(t)}{1 + b(t)}, \tag{52}$$

where:

$$a(t) = \exp\left[\int_s^t \alpha(s')ds'\right], \tag{53}$$

$$b(t) = \frac{1}{2}\int_s^t ds'\, \chi_2'(s')\, \exp\left[\int_{s'}^t \alpha(s'')ds''\right]. \tag{54}$$

Inserting $a(t)$ and $b(t)$ into Eq.(52) and comparing with Eq.(45) immediately establishes the equivalence to the survival probability obtained using the backward Master equation.

When the medium contains a random source, the forward Master equation gives an explicit solution for the survival probability only for static reactivity [8] and is given by:

$$\mathcal{P}_{\mathcal{S}}(t|t_0) = 1 - [1 + b(t)]^{-\eta}, \tag{55}$$

where $b(t)$ follows from Eq.(54) for constant χ_2' and α:

$$\begin{aligned} b(t) &= \frac{\chi_2'}{2\alpha}\left[\exp\alpha\left(t - t_0\right) - 1\right], \\ &= \frac{1}{POI}\left[\exp\alpha\left(t - t_0\right) - 1\right]. \end{aligned} \tag{56}$$

Inserting Eq.(56) into Eq.(55) and comparing with Eq.(51) demonstrates the equivalence of the survival probabilities in the backward and forward formulations also in the case of a medium containing a random source.

7 Numerical Considerations

For convenience, we recall the equations that are pertinent for the numerical computation of the probabilities of interest, namely, Eqs.(27a) – (27b) for the single chain case:

$$-\frac{\partial P(t|s)}{\partial s} = \alpha(s)P(t|s) - \frac{p_f(s)}{\tau}\sum_{k=2}^{\nu_{max}} (-1)^k \frac{\chi_k}{k!} P^k(t|s), \tag{57a}$$

$$\lim_{s\to t} P(t|s) = 1, \tag{57b}$$

and Eqs.(37a) – (37b) for the extinction probability when a random intrinsic source is present:

$$-\frac{\partial \Theta_0(t|s)}{\partial s} = \mathcal{S}\left[\sum_{k=1}^{\nu_{max}} \frac{(-1)^k}{k!}\chi_k^s P^k(t|s)\right]\Theta_0(t|s), \tag{58a}$$

$$\lim_{s\to t} \Theta_0(t|s) = 1. \tag{58b}$$

We stress that the source multiplicities (or factorial moments) are not necessarily the same as those for induced fission appearing in Eq.(57a). If the source is due to spontaneous fission the two multiplicities may in fact be identical, but in general this is not the case. Eq.(57a) is a stand-alone first-order nonlinear ordinary differential equation of degree ν_{max} for the single chain survival probability and can be readily solved using standard ode solvers. Those based on backward-difference formulae of various orders of accuracy and degrees of stiffness are perhaps optimal and a convenient selection of such solvers are available in MATLAB. Our derivation above has yielded a backward-in-time formulation, so that the solution must be obtained by integrating from a final time t backwards to an arbitrary earlier time. However, it may be expedient to first convert Eqs.(57a) – (57b) to initial value form using the change of variable $t' = t - s \geq 0$, with t' now measuring the time since the insertion of the initial neutron and with the origin at $t' = 0$. Note that when the fission probability and hence alpha vary with time, the solution will depend additionally but parametrically on the final time t. This is not the case in the time independent case.

The generalized Bartlett formula given by Eq.(38) directly yields the extinction probability when a source is present, by a numerical integration over the single chain survival probability and the source (if the source strength is time varying). However, this requires applying a quadrature rule to a time-discretized survival probability, which may limit the accuracy of the computed extinction probability. A more accurate and efficient approach is to numerically solve the linear differential equation describing the source extinction probability given by Eqs.(58a) – (58b) in conjunction with that for the single-chain survival probability. This is readily done within the same code and certainly very conveniently so in MATLAB. Such numerical implementation is presently ongoing and we hope to soon report on results under different reactivity and source conditions as well as a detailed assessment of the affect of uncertainty in the neutron multiplicities and lifetime on the survival and extinction probabilities.

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