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Monte-Carlo Generation of Time Evolving Fission Chains

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1 Introduction

About a decade ago, a computer code was written to model neutrons from their “birth” to their final “death” in thermal neutron detectors (^3He tubes): SrcSim had enough physics to track the neutrons in multiplying systems, appropriately increasing and decreasing the neutron population as they interacted by absorption, fission and leakage. The theory behind the algorithms assumed that all neutrons produced in a fission chain were all produced simultaneously, and then diffused to the neutron detectors. For cases where the diffusion times are long compared to the fission chains, SrcSim is very successful. Indeed, it works extraordinarily well for thermal neutron detectors and bare objects, because it takes tens of microseconds for fission neutrons to slow down to thermal energies, where they can be detected. Microseconds are a very long time compared to the lengths of the fission chains. However, this inherent assumption in the theory prevents its use to cases where either the fission chains are long compared to the neutron diffusion times (water-cooled nuclear reactors, or heavily moderated object, where the theory starts failing), or the fission neutrons can be detected shortly after they were produced (fast neutron detectors). For these cases, a new code needs to be written, where the underlying assumption is not made.

The purpose of this report is to develop an algorithm to generate the arrival times of neutrons in fast neutron detectors, starting from a neutron source such as a spontaneous fission source (^{252}Cf) or a multiplying source (Pu). This code will be an extension of SrcSim to cases where correlations between neutrons in the detectors are on the same or shorter time scales as the fission chains themselves.

2 Rate equation for the internal neutron population

We will start from the rate equation given in [1]. The probability of obtaining n neutrons in the system at time $t + \Delta t$ is determined from the number of neutrons at time t :

$$\mathcal{P}_n(t + \Delta t) = \left(1 - n \frac{\Delta t}{\tau}\right) \mathcal{P}_n(t) + q(n+1) \frac{\Delta t}{\tau} \mathcal{P}_{n+1}(t) + p \sum_{\nu=0}^8 (n+1-\nu) \frac{\Delta t}{\tau} C_\nu \mathcal{P}_{n+1-\nu}(t) \quad (1)$$

where $q = 1 - p$ is the probability for a neutron to leak out of the medium or to be absorbed without inducing a subsequent fission.

3 From the rate equation to a Monte-Carlo algorithm

In a Monte-Carlo simulation of a fission chain, we know the number of neutrons we have at time t , let's say n . For Δt small compared to τ , we calculate the number of neutrons at time $t + \Delta t$ based on an equation

which gives us the probabilities of something or “events” occurring. Eq. 1 is not in the right form for Monte-Carlo sampling, because it does not give us the probabilities that “events” will occur starting with n neutrons. We will manipulate the indices of Eq. 1 so that it gives us the probabilities of obtaining some numbers of neutrons at time $t + \Delta t$, starting with n neutrons at time t . If one has n neutrons in the system at time t , the probability of getting $n - 1$ neutrons in the system at time $t + \Delta t$ is

$$\mathcal{P}_{n-1}(t + \Delta t) = qn \frac{\Delta t}{\tau} \mathcal{P}_n(t) + pn \frac{\Delta t}{\tau} C_0 \mathcal{P}_n(t) \quad (2)$$

$qn \frac{\Delta t}{\tau}$ in the first term on the right side of the equation represents the probability of losing one of the n initial neutrons to either leakage or absorption by a nucleus without fissioning it. $pn \frac{\Delta t}{\tau} C_0$ in the second term represents the probability that one of the initial n neutrons fissions a nucleus and does not produce any fission neutrons. Starting with the same internal neutron population of n neutrons at time t , the probability of getting n neutrons in the system at time $t + \Delta t$ is

$$\mathcal{P}_n(t + \Delta t) = \left(1 - n \frac{\Delta t}{\tau}\right) \mathcal{P}_n(t) + pn \frac{\Delta t}{\tau} C_1 \mathcal{P}_n(t) \quad (3)$$

$(1 - n \frac{\Delta t}{\tau})$ in the first term on the right side of the equation represents the probability that none of the n initial neutrons interacts with matter in the time period Δt . $pn \frac{\Delta t}{\tau} C_1$ in the second term represents the probability that one of the n initial neutrons fissions a nucleus and produces a single fission neutron. The probability of getting $n + 1$ neutrons in the system at time $t + \Delta t$ is

$$\mathcal{P}_{n+1}(t + \Delta t) = pn \frac{\Delta t}{\tau} C_2 \mathcal{P}_n(t) \quad (4)$$

where $pn \frac{\Delta t}{\tau} C_2$ is the probability that one of the n initial neutrons fissions a nucleus and produces two fission neutrons. And so on for fissions producing more neutrons.

In summary, the time-dependent probabilities of getting $n - 1$ through $n + v - 1$ neutrons at time $t + \Delta t$ starting with an internal neutron population of n neutrons at time t is given by

$$\begin{cases} \mathcal{P}_{n-1}(t + \Delta t) &= (qn \frac{\Delta t}{\tau} + pn \frac{\Delta t}{\tau} C_0) \mathcal{P}_n(t) \\ \mathcal{P}_n(t + \Delta t) &= ((1 - n \frac{\Delta t}{\tau}) + pn \frac{\Delta t}{\tau} C_1) \mathcal{P}_n(t) \\ \mathcal{P}_{n+v-1}(t + \Delta t) &= pn \frac{\Delta t}{\tau} C_v \mathcal{P}_n(t) \end{cases} \quad \text{for } 2 \leq v \leq 8 \quad (5)$$

The probabilities for the system to transition from n neutrons to a different number of neutrons is given by

$$\begin{cases} \frac{\mathcal{P}_{n-1}(t+\Delta t)}{\mathcal{P}_n(t)} &= qn \frac{\Delta t}{\tau} + pn \frac{\Delta t}{\tau} C_0 \\ \frac{\mathcal{P}_n(t+\Delta t)}{\mathcal{P}_n(t)} &= (1 - n \frac{\Delta t}{\tau}) + pn \frac{\Delta t}{\tau} C_1 \\ \frac{\mathcal{P}_{n+v-1}(t+\Delta t)}{\mathcal{P}_n(t)} &= pn \frac{\Delta t}{\tau} C_v \end{cases} \quad \text{for } 2 \leq v \leq 8 \quad (6)$$

The right side of the first sub-equation in Eq. 6 gives the probability that the number of neutrons will decrease by 1 between t and $t + \Delta t$. There are two possible causes for this decrease: a neutron can either (a) be absorbed by a nucleus or leak out of the medium (with probability $qn \frac{\Delta t}{\tau}$), or (b) fission and produce no fission neutrons (with probability $pn \frac{\Delta t}{\tau} C_0$).

The right side of the second sub-equation in Eq. 6 gives the probability that the number of neutrons does not change between t and $t + \Delta t$, this can be the result of two causes: either none of the n neutrons interacted with matter (with probability $(1 - n \frac{\Delta t}{\tau})$), or 1 of the n initial neutrons fissioned a nucleus (with probability $pn \frac{\Delta t}{\tau} C_1$), which in turn “evaporated” a single fission neutron.

If we are interested in computing the number of fissions that occurred in the chain, it is important to treat the different physical events in the first and second sub-equations in Eq. 6 separately.

The probability f_{event} that anything happens in the time window t to $t + dt$ — as opposed to nothing happening (with probability $(1 - n\frac{\Delta t}{\tau})$) — is given by:

$$\begin{aligned}
f_{\text{event}} &= \frac{\sum_{\Delta n=-1}^7 \mathcal{P}_{n+\Delta n}(t+\Delta t)}{\mathcal{P}_n(t)} - \left(1 - n\frac{\Delta t}{\tau}\right) \\
&= \frac{\sum_{\Delta n=-1}^7 \mathcal{P}_{n+\Delta n}(t+\Delta t)}{\mathcal{P}_n(t)} \\
&= \frac{qn\frac{\Delta t}{\tau} + pn\frac{\Delta t}{\tau} \sum_{v=0}^8 \mathcal{C}_v}{qn\frac{\Delta t}{\tau} + \left(1 - n\frac{\Delta t}{\tau}\right) + pn\frac{\Delta t}{\tau} \sum_{v=0}^8 \mathcal{C}_v} \\
&= \frac{qn\frac{\Delta t}{\tau} + pn\frac{\Delta t}{\tau}}{qn\frac{\Delta t}{\tau} + \left(1 - n\frac{\Delta t}{\tau}\right) + pn\frac{\Delta t}{\tau}} \\
&= n\frac{\Delta t}{\tau}
\end{aligned} \tag{7}$$

One should note that f_{event} is independent of t , which is true as long as Δt is small compared to τ .

To advance the fission chain by one small Δt step — where Δt is small compared to τ —, typical Monte-Carlo algorithms compute the probability that an event happens in the time windows t to $t + \Delta t$. In our case, the Monte-Carlo algorithm will “throw the dice” and generate a random number θ between 0 and 1. If θ is greater than f_{event} , nothing will happen in that time step, and the algorithm will proceed to the next time step. If θ is between 0 and f_{event} , a reaction took place. The algorithm will then proceed to determine which one of the reactions took place. The probabilities for specific reactions to happen in the time window t to $t + \Delta t$ can be written as

$$\left\{ \begin{array}{l} f_{\text{loss}} \\ f_{\text{fiss. } v \text{ neutrons}} \end{array} \right. = \begin{array}{l} = \frac{qn\frac{\Delta t}{\tau}}{qn\frac{\Delta t}{\tau} + \left(1 - n\frac{\Delta t}{\tau}\right) + pn\frac{\Delta t}{\tau} \sum_{v=0}^8 \mathcal{C}_v} \\ = qn\frac{\Delta t}{\tau} \\ = \frac{pn\frac{\Delta t}{\tau} \mathcal{C}_v}{qn\frac{\Delta t}{\tau} + \left(1 - n\frac{\Delta t}{\tau}\right) + pn\frac{\Delta t}{\tau} \sum_{v=0}^8 \mathcal{C}_v} \\ = pn\frac{\Delta t}{\tau} \mathcal{C}_v \end{array} \tag{8}$$

If θ is between 0 and f_{loss} , one neutron will be lost by absorption or leakage, the internal number population will decrease by 1. If $f_{\text{loss}} \leq \theta < f_{\text{loss}} + f_{\text{fiss. } 0 \text{ neutrons}}$, one neutron caused a fission with no fission neutrons produced, the number of neutrons in the internal population will decrease by 1. The changes in number of neutrons in the internal population can be summarized by

$$n(t + \Delta t) = \begin{cases} n(t) - 1 & \text{for } 0 \leq \theta \leq f_{\text{loss}} \\ n(t) + \Delta n & \text{for } f_{\text{loss}} + \sum_{i=0}^{\Delta n} f_{\text{fiss. } i \text{ neutrons}} < \theta \leq f_{\text{loss}} + \sum_{i=0}^{\Delta n+1} f_{\text{fiss. } i \text{ neutrons}} \\ n(t) & \text{for } \theta > f_{\text{loss}} + \sum_{i=0}^8 f_{\text{fiss. } i \text{ neutrons}} \end{cases} \tag{9}$$

where Δn is the number of neutrons by which the internal population changes between t and $t + dt$. Δn can take any value between -1 and 7, inclusively. Using the definitions of f_{loss} and $f_{\text{fiss. } v \text{ neutrons}}$ explicitly, we

can write

$$n(t + \Delta t) = \begin{cases} n(t) - 1 & \text{for } 0 \leq \theta \leq qn \frac{\Delta t}{\tau} \\ n(t) + \Delta n & \text{for } qn \frac{\Delta t}{\tau} + pn \frac{\Delta t}{\tau} \sum_{i=0}^{\Delta n} C_i < \theta \leq qn \frac{\Delta t}{\tau} + pn \frac{\Delta t}{\tau} \sum_{i=0}^{\Delta n+1} C_i \text{ for } -1 \leq \Delta n \leq 7 \\ n(t) & \text{for } \theta > n \frac{\Delta t}{\tau} \end{cases} \quad (10)$$

While there are two equations to decrease the internal neutron population by 1, they correspond to two different physical events. Eq. 10 can be reduced to a single equation

$$n(t + \Delta t) = n(t) + \begin{cases} \Delta n & \text{for } \theta \begin{cases} > qn \frac{\Delta t}{\tau} H[\Delta n] + pn \frac{\Delta t}{\tau} \sum_{i=0}^{\Delta n} C_i \\ \leq qn \frac{\Delta t}{\tau} H[\Delta n + 1] + pn \frac{\Delta t}{\tau} \sum_{i=0}^{\Delta n+1} C_i \end{cases} \\ 0 & \text{for } \theta > n \frac{\Delta t}{\tau} \end{cases} \quad (11)$$

where $H[n]$ is a step function, also known as the discrete Heaviside function defined as

$$H[n] = \begin{cases} 0, & n < 0, \\ 1, & n \geq 0, \end{cases} \quad (12)$$

where n is an integer. Unfortunately, using this last equation directly does not distinguish the two different ways of losing one neutron in the time step Δt .

4 Onto a more efficient Monte-Carlo algorithm

While this works when the time step Δt is small compared to τ , it fails for larger Δt , because these equations were derived with the assumption of Δt small compared to τ . This can easily be seen for the probability $(1 - n \frac{\Delta t}{\tau})$ that none of the n neutrons interacted with matter will eventually become negative for large Δt , which is unphysical.

Using small Δt time steps can become prohibitively expensive. For most time steps, nothing will happen, and we will move on to the next time step. We can use a faster algorithm. Instead of generating a random number θ and compare it with the probabilities 6 and 7 for a small Δt , we could determine the required time step size Δt for an event to happen. Let us rewrite the time-dependent probabilities 5 for the internal neutron population to change from n neutrons at time t to a different number of neutrons at time $t + dt$ in a more accurate way.

Revisiting the probabilities $\mathcal{P}_n(t + \Delta t)$ in the rate equation 1, we see that instead of using $(1 - n \frac{\Delta t}{\tau})$ for the survival probability of the n neutrons between t and $t + \Delta t$, it is more accurate to use a different expression, from which the approximation $(1 - n \frac{\Delta t}{\tau})$ was derived. The survival probability of a single neutron between t and $t + \Delta t$ is given by $\mathcal{P}_0(\frac{\Delta t}{\tau}) = e^{-\frac{\Delta t}{\tau}}$, i.e. the Poisson probability that 0 event will occur in Δt given the average event frequency $\frac{1}{\tau}$. The survival probability of n neutrons between t and $t + \Delta t$ is thus simply $(\mathcal{P}_0(\frac{\Delta t}{\tau}))^n = e^{-n \frac{\Delta t}{\tau}}$. We easily see that this new expression reduces to $(1 - n \frac{\Delta t}{\tau})$ for small Δt compared to τ . Moreover, it is not an approximation, it is valid for both small and large $\frac{\Delta t}{\tau}$, and does not become negative for large $\frac{\Delta t}{\tau}$. Similarly, we can use Poisson probabilities for the other terms as well. The

new rate equation reads

$$\begin{aligned} \mathcal{P}_n(t + \Delta t) &= \left(e^{-\frac{\Delta t}{\tau}}\right)^n \mathcal{P}_n(t) + q \binom{n+1}{1} \left(1 - e^{-\frac{\Delta t}{\tau}}\right) \left(e^{-\frac{\Delta t}{\tau}}\right)^n \mathcal{P}_{n+1}(t) \\ &\quad + p \sum_{v=0}^8 \binom{n+1-v}{1} \left(1 - e^{-\frac{\Delta t}{\tau}}\right) \left(e^{-\frac{\Delta t}{\tau}}\right)^{n-v} \mathcal{C}_v \mathcal{P}_{n+1-v}(t) \end{aligned} \quad (13)$$

where the second term is the probability that out of $n + 1$ neutrons, n will not leak out, nor be absorbed, and 1 will leak out. There are $n + 1$ ways of choosing 1 neutron out of $n + 1$, so the factor $\binom{n+1}{1}$. The third term is to be interpreted similarly.

We can follow the same logical steps as previously to compute the time-dependent probabilities of getting $n - 1$ through $n + v - 1$ neutrons at time $t + \Delta t$ starting with an internal neutron population of n neutrons at time t . These new equations are the counterparts of Eq. 5:

$$\begin{cases} \mathcal{P}_{n-1}(t + \Delta t) &= (qn + pn\mathcal{C}_0) \left(1 - e^{-\frac{\Delta t}{\tau}}\right) \mathcal{P}_n(t) \\ \mathcal{P}_n(t + \Delta t) &= \left(e^{-n\frac{\Delta t}{\tau}} + pn \left(1 - e^{-\frac{\Delta t}{\tau}}\right) \mathcal{C}_1\right) \mathcal{P}_n(t) \\ \mathcal{P}_{n+v-1}(t + \Delta t) &= pn \left(1 - e^{-\frac{\Delta t}{\tau}}\right) \mathcal{C}_v \mathcal{P}_n(t) \end{cases} \quad \text{for } 2 \leq v \leq 8 \quad (14)$$

The probabilities for the system to transition from n neutrons to a different number of neutrons is simply the above expressions divided by $\mathcal{P}_n(t)$, as we did previously for Eq. 6:

$$\begin{cases} \frac{\mathcal{P}_{n-1}(t+\Delta t)}{\mathcal{P}_n(t)} &= (qn + pn\mathcal{C}_0) \left(1 - e^{-\frac{\Delta t}{\tau}}\right) \\ \frac{\mathcal{P}_n(t+\Delta t)}{\mathcal{P}_n(t)} &= e^{-n\frac{\Delta t}{\tau}} + pn\mathcal{C}_1 \left(1 - e^{-\frac{\Delta t}{\tau}}\right) \\ \frac{\mathcal{P}_{n+v-1}(t+\Delta t)}{\mathcal{P}_n(t)} &= pn\mathcal{C}_v \left(1 - e^{-\frac{\Delta t}{\tau}}\right) \end{cases} \quad \text{for } 2 \leq v \leq 8 \quad (15)$$

Using these new expressions for the $\mathcal{P}_n(t + \Delta t)$'s, we can now write the survival probability f_{survival} that nothing happens to the n neutrons in the time window t to $t + \Delta t$:

$$f_{\text{survival}}(t + \Delta t) = e^{-n\frac{\Delta t}{\tau}} \quad (16)$$

Given the random number θ , we can determine Δt by equating Eq. 16 to θ . This time step Δt will be such that nothing will have happened in the time window t to $t + \Delta t$. We will then use another random number θ' to check which specific event occurred at time $t + \Delta t$. For that purpose, we will now compute the probabilities for specific reactions to happen at time $t + \Delta t$:

$$\begin{cases} f_{\text{loss}}(t + \Delta t) &= \frac{qn}{qn + pn \sum_{i=0}^8 \mathcal{C}_i} = q \\ f_{\text{fiss. } v \text{ neutrons}}(t + \Delta t) &= \frac{pn\mathcal{C}_v}{qn + pn \sum_{i=0}^8 \mathcal{C}_i} = p\mathcal{C}_v \end{cases} \quad (17)$$

The changes in number of neutrons in the internal population at time $t + \Delta t$ can be summarized by

$$n(t + \Delta t) = \begin{cases} n(t) - 1 & \text{for } 0 \leq \theta' \leq q \\ n(t) + \Delta n & \text{for } q + p \sum_{i=0}^{\Delta n} \mathcal{C}_i \mathcal{P}_n(t) < \theta' \leq q + p \sum_{i=0}^{\Delta n+1} \mathcal{C}_i \end{cases} \quad (18)$$

or

$$n(t + \Delta t) = n(t) + \Delta n \text{ for } \theta' \begin{cases} > H[\Delta n]q + p \sum_{i=0}^{\Delta n} C_i \\ \leq H[\Delta n + 1]q + p \sum_{i=0}^{\Delta n + 1} C_i \end{cases} \quad (19)$$

Δn is the number of neutrons by which the internal population changes between t and $t + \Delta t$, Δn can take any value between -1 and 7, inclusively.

While we could use the equations above in a Monte-Carlo simulation to track n neutrons at once, tracking a single neutron at a time has some advantages. In terms of algorithm implementation, treating a single neutron at a time leads to a recursive algorithm, where each fission branch is followed all the way to the leaves before moving to the next fission branch. In this case, some of the first detected neutrons produced by the recursion could be detected last, i.e. neutrons are not produced in chronological order by the algorithm. On the other hand, treating the entire population of n neutrons at once leads to following all the branches at once. Consequently, neutrons are produced in chronological order by the non-recursive algorithm.

Tracking a single neutron at a time is paramount to treating each neutron as a singleton neutron population as soon as it is generated. While the Eqs. 17 that determine the destiny of a neutron does not change in this case, Eq. 16 becomes

$$f_{\text{survival}}(t + \Delta t) = e^{-\frac{\Delta t}{\tau}} \quad (20)$$

for a neutron population of 1. The time constant τ is the total neutron lifetime that determines the time scale for the time evolution of each neutron and thus of the fission chain. For each neutron, the time between events is determined from the Poisson probability to have a time gap, $e^{-t/\tau}$. The probability that a neutron survives without interaction for a time u , and then has an interaction within du is given by

$$\int_0^t e^{-\frac{u}{\tau}} \frac{du}{\tau} = 1 - e^{-\frac{t}{\tau}} \quad (21)$$

where $\frac{du}{\tau}$ is the neutron interaction probability in a small time window du . The time interval t is determined by equating the cumulative distribution to a random number θ , between 0 and 1,

$$t = -\tau \ln(1 - \theta) \quad (22)$$

After the time t , Eqs. 17 are used: either the neutron is lost with probability q , or the neutron induces a fission with probability p . This decision is determined by a random number. If fission is selected, the number of emitted neutrons is sampled from the probability distribution, C_v . The times of each event are recorded.

5 Detection of neutrons

We have so far focused our attention on the internal neutron population. However, we are also interested in the detection of neutrons by our detectors. Every time a neutron is lost (f_{loss} in Eq. 8 and Eq. 17), the algorithm will decide whether the lost neutron is detected. The detection probability of a lost neutron is ε . $1 - \varepsilon$ represents the probability for a lost neutron to go undetected.

For thermal neutron detection, it often takes times of the order of microseconds for fast neutrons to thermalize. While we could in principle include a delay between the last neutron interaction in the system and its detection using a thermalization time constant, we will consider here that neutrons are immediately detected after their last interaction in the material. This is a reasonable approximation for fast neutron detectors.

6 Reconstruction of neutron and fission populations

For fission chains initiated by single neutrons, the evolutions of the populations of internal neutrons, external neutrons and fissions as a function of time are given analytically in Ref. [2]. To briefly summarize, the fission chain distribution $P_{k,m,s}(t)$ tracks the populations of internal neutrons k , of neutrons that have escaped from the evolving chain m , and of fissions s , starting with a fission chain initiated by a single neutron. Taking derivatives with respect to x , y and z of its generating function

$$f(t, x, y, z) = \sum_{k=0}^{\infty} \sum_{m=0}^{\infty} \sum_{s=0}^{\infty} P_{k,m,s}(t) x^k y^m z^s, \quad (23)$$

and setting the different population variables to unity, we can obtain the moments of the different populations.

For instance, the first 3 combinatorial moments of the internal neutron population are given by

$$\left\{ \begin{array}{l} \frac{\partial f}{\partial x} = e^{-\alpha t} \\ \frac{1}{2} \frac{\partial^2 f}{\partial x^2} = \frac{M-1}{\bar{v}} v_2 e^{-\alpha t} (1 - e^{-\alpha t}) \\ \frac{1}{3!} \frac{\partial^3 f}{\partial x^3} = \left(\frac{M-1}{\bar{v}} v_2 \right)^2 e^{-\alpha t} (1 - 2e^{-\alpha t} + e^{-2\alpha t}) + \frac{1}{2} \frac{M-1}{\bar{v}} v_3 e^{-\alpha t} (1 - e^{-2\alpha t}) \end{array} \right. \quad (24)$$

where y and z were set to 1.

To check the equations against our code, we ran a Monte-Carlo simulation of a large number of fission chains, and kept track of the number of internal neutrons in the system as a function of time. The simulated system was a random source emitting a single neutron at a time, the multiplying isotope was ^{235}U , it multiplied with a multiplication of $M=10$. The distribution of numbers of fission neutrons for the induced fission of ^{235}U was coming from nuclear data evaluated at 1 MeV. The average time τ it takes for a neutron to disappear in the medium was set to 10 ns.

The red markers with error bars in Fig. 1 shows the results of this simulation along with the moments given by the above Eqs. 24 in green. We observe that the analytical equations precisely track the Monte-Carlo results.

As for the external neutron population, that is the population of neutrons that are detected, the first 3 combinatorial moments of that neutron population are

$$\left\{ \begin{array}{l} \frac{\partial f}{\partial y} = qM(1 - e^{-\alpha t}) \\ \frac{1}{2} \frac{\partial^2 f}{\partial y^2} = (qM)^2 \frac{M-1}{\bar{v}} v_2 (1 - 2\alpha t e^{-\alpha t} - e^{-2\alpha t}) \\ \frac{1}{3!} \frac{\partial^3 f}{\partial y^3} = \frac{1}{2} (qM)^3 \frac{M-1}{\bar{v}} v_3 (2 + (3 - 6\alpha t) e^{-\alpha t} - 6e^{-2\alpha t} + e^{-3\alpha t}) \\ \quad + (qM)^3 \left(\frac{M-1}{\bar{v}} v_2 \right)^2 \left(2 - (2(\alpha t)^2 + 2\alpha t - 1) e^{-\alpha t} - (2 + 4\alpha t) e^{-2\alpha t} - e^{-3\alpha t} \right) \end{array} \right. \quad (25)$$

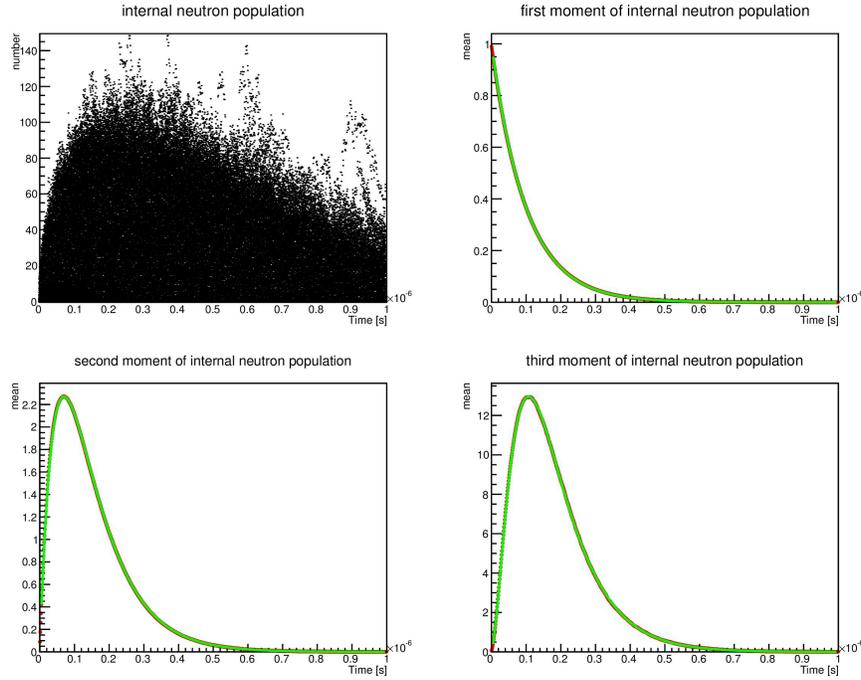


Figure 1: Time evolution of the internal neutron population with its 3 first moments. The Monte-Carlo simulation was a random source emitting single neutrons, the multiplying isotope was ^{235}U of multiplication 10. The nuclear data for the induced fission of ^{235}U were evaluated at 1 MeV. $\tau=10$ ns, source strength=1000 neutrons/sec, data time=12 hours.

Fig. 2 shows the moments given by the above Eqs. 25, along with the Monte-Carlo simulation results in red. A detection efficiency of 100% was used for both the simulation and the equations. Again, the analytical equations track the Monte-Carlo results within the uncertainty. In the first quadrant of Fig. 2, it is interesting to note the lonely track: a particularly large fission chain produced a huge fluctuation in terms of numbers of neutrons detected.

Lastly, the first 3 combinatorial moments of the fission population, i.e. the number of fissions, are given

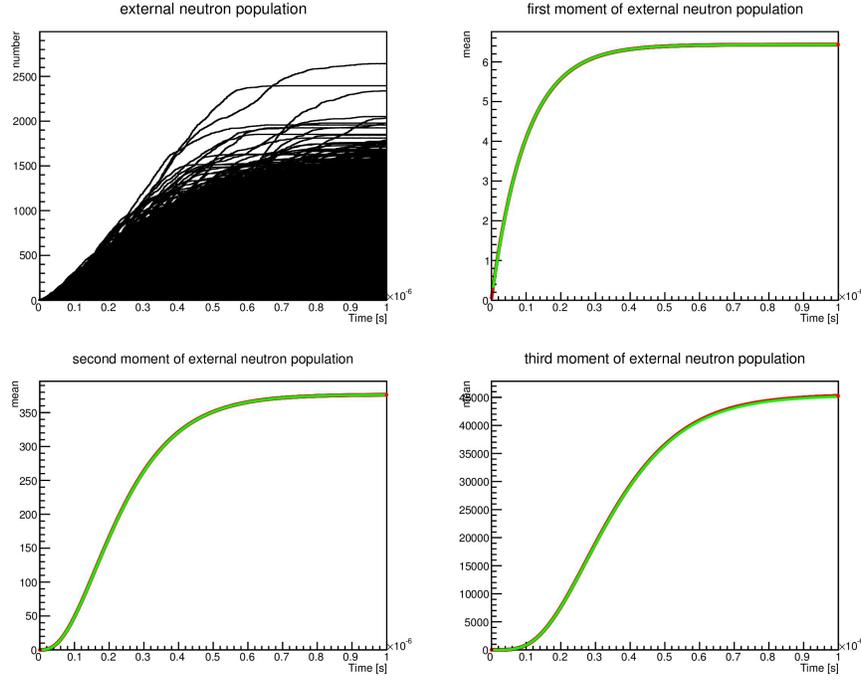


Figure 2: Time evolution of the external neutron population with its 3 first moments. The Monte-Carlo simulation was a random source emitting single neutrons, the multiplying isotope was ^{235}U of multiplication 10. The nuclear data for the induced fission of ^{235}U were evaluated at 1 MeV. $\tau=10$ ns, detection efficiency $\varepsilon=100\%$, source strength=1000 neutrons/sec, data time=12 hours.

by these 3 equations:

$$\left\{ \begin{array}{l}
 \frac{\partial f}{\partial z} = M(1 - e^{-\alpha t}) \\
 \frac{1}{2} \frac{\partial^2 f}{\partial z^2} = \left(\frac{M-1}{\bar{v}} \right)^2 \frac{M-1}{\bar{v}} v_2 (1 - 2\alpha t e^{-\alpha t} - e^{-2\alpha t}) + \left(\frac{M-1}{\bar{v}} \right)^2 \bar{v} (1 - e^{-\alpha t} - \alpha t e^{-\alpha t}) \\
 \frac{1}{3!} \frac{\partial^3 f}{\partial z^3} = \left(\frac{M-1}{\bar{v}} \right)^3 v_2 (1 - 2\alpha t e^{-\alpha t} - e^{-2\alpha t}) + \left(\frac{M-1}{\bar{v}} \right)^3 \bar{v}^2 (1 - e^{-\alpha t}) \left(1 + \alpha t + \frac{1}{2} (\alpha t)^2 \right) \\
 \quad + \left(\frac{M-1}{\bar{v}} \right)^3 (M-1) v_2 \left(3 - 3e^{-2\alpha t} - 2\alpha t e^{-2\alpha t} - 4\alpha t e^{-\alpha t} - 2(\alpha t)^2 e^{-\alpha t} \right) \\
 \quad + \left(\frac{M-1}{\bar{v}} \right)^3 \frac{M-1}{\bar{v}} v_3 \left(1 + \frac{1}{2} e^{-3\alpha t} - 3e^{-2\alpha t} + \frac{3}{2} e^{-\alpha t} - 3\alpha t e^{-\alpha t} \right) \\
 \quad + \left(\frac{M-1}{\bar{v}} \right)^3 \left(\frac{M-1}{\bar{v}} v_2 \right)^2 \left(2 - e^{-3\alpha t} - 2e^{-2\alpha t} - 4\alpha t e^{-2\alpha t} + e^{-\alpha t} - 2\alpha t e^{-\alpha t} - 2(\alpha t)^2 e^{-\alpha t} \right)
 \end{array} \right. \quad (26)$$

Fig. 3 shows the simulation results in red along with the moments given by the Eqs. 26 in green. Again, the analytical equations track the Monte-Carlo results.

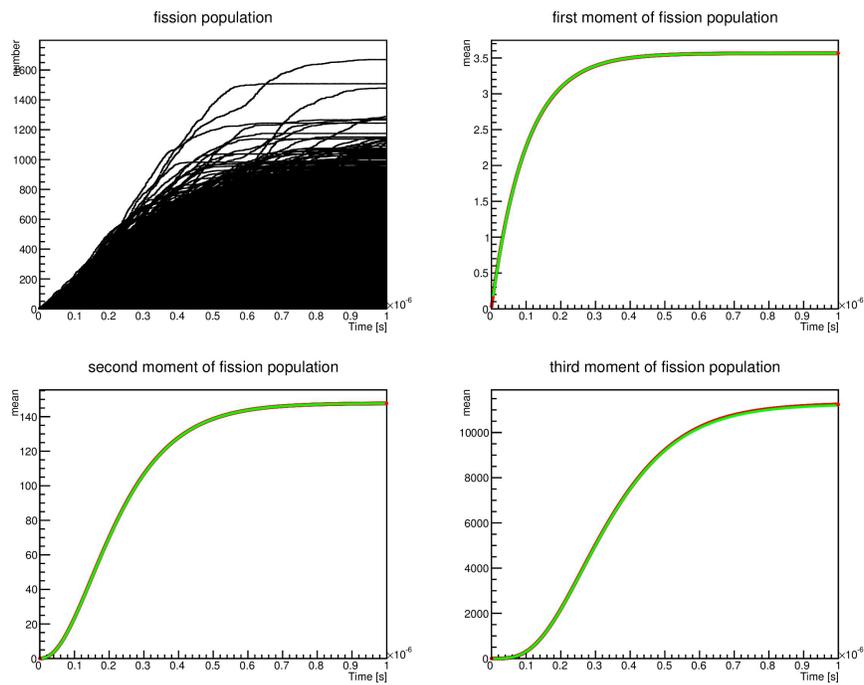


Figure 3: Time evolution of the fission population with its 3 first moments. The Monte-Carlo simulation was a random source emitting single neutrons, the multiplying isotope was ^{235}U of multiplication 10. The nuclear data for the induced fission of ^{235}U were evaluated at 1 MeV. $\tau=10$ ns, source strength=1000 neutrons/sec, data time=12 hours.

One can also calculate correlations between different populations of the time-evolving fission chain. The moments of the correlated internal neutron and fission population are

$$\left\{ \begin{array}{l}
 \frac{\partial^2 f}{\partial x \partial z} = (M-1) \alpha t e^{-\alpha t} + 2 \left(\frac{M-1}{\bar{\nu}} \right)^2 v_2 (e^{-2\alpha t} + \alpha t e^{-\alpha t} - e^{-\alpha t}) \\
 \\
 \frac{1}{2} \frac{\partial^3 f}{\partial x^2 \partial z} = \left(\frac{M-1}{\bar{\nu}} \right) v_2 e^{-\alpha t} (1 - e^{-\alpha t}) + \left(\frac{M-1}{\bar{\nu}} \right)^2 \bar{\nu} v_2 e^{-\alpha t} (1 + \alpha t - e^{-\alpha t} - 2\alpha t e^{-\alpha t}) \\
 \quad + 3 \left(\frac{M-1}{\bar{\nu}} \right)^2 v_3 e^{-\alpha t} (0.5 - e^{-\alpha t} + 0.5 e^{-2\alpha t}) \\
 \quad + \left(\frac{M-1}{\bar{\nu}} \right)^3 v_2^2 e^{-\alpha t} (2\alpha t - 1 + 4e^{-\alpha t} - 4\alpha t e^{-\alpha t} - 3e^{-2\alpha t}) \\
 \\
 \frac{1}{2} \frac{\partial^3 f}{\partial x \partial z^2} = (M-1)^2 e^{-\alpha t} \left[\frac{(\alpha t)^2}{2} + \left(\frac{M-1}{\bar{\nu}} \right) D_2 (2 - 2e^{-\alpha t} + \alpha t (\alpha t - 2)) \right] \\
 \quad + \frac{1}{2} e^{-\alpha t} \left(\frac{M-1}{\bar{\nu}} \right)^2 \bar{\nu} \left[4D_2 (\alpha t - 1 + e^{-\alpha t}) + 3D_3 \left(\frac{M-1}{\bar{\nu}} \right) (-e^{-2\alpha t} + 4e^{-\alpha t} + 2\alpha t - 3) \right. \\
 \quad + 2D_2 v_2 \left(\frac{M-1}{\bar{\nu}} \right)^2 (3e^{-2\alpha t} + 8\alpha t e^{-\alpha t} - 3 + 2\alpha t (\alpha t - 1)) \\
 \quad \left. + 2 \left(\frac{M-1}{\bar{\nu}} \right) v_2 (6e^{-\alpha t} + 4\alpha t e^{-\alpha t} - 6 + \alpha t (2 + \alpha t)) \right]
 \end{array} \right. \tag{27}$$

Fig. 4 shows the simulation results in red along with the moments given by Eqs. 27 in green.

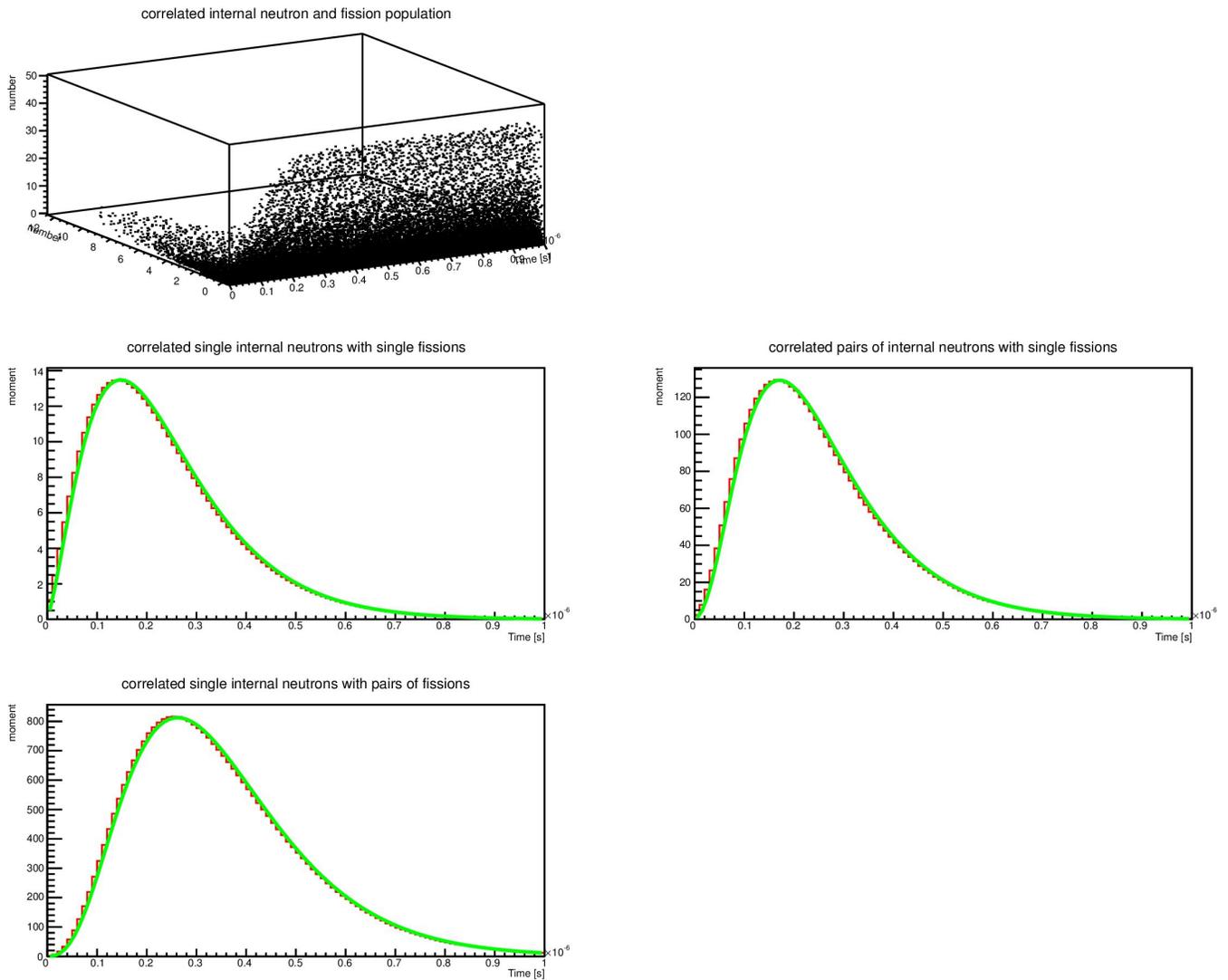


Figure 4: Time evolution of the correlated internal neutron population and fission population. The Monte-Carlo simulation was a random source emitting single neutrons, the multiplying isotope was ^{235}U of multiplication 10. The nuclear data for the induced fission of ^{235}U were evaluated at 1 MeV. $\tau=10$ ns, 1000 neutrons/sec, data time=12 hours.

The moments of the correlated internal neutron and external neutron populations are

$$\left\{ \begin{array}{l} \frac{\partial^2 f}{\partial x \partial y} = 2 \left(M - \frac{M-1}{\bar{v}} \right) (M-1) D_2 ((\alpha t - 1) e^{-\alpha t} + e^{-2\alpha t}) \\ \frac{1}{2} \frac{\partial^3 f}{\partial x^2 \partial y} = \left(M - \frac{M-1}{\bar{v}} \right) ((M-1) D_2)^2 ((2\alpha t - 1) e^{-\alpha t} + 4(1 - \alpha t) e^{-2\alpha t} - 3e^{-3\alpha t}) \\ \quad + \frac{3}{2} \left(M - \frac{M-1}{\bar{v}} \right) (M-1) D_3 (e^{-\alpha t} - 2e^{-2\alpha t} + e^{-3\alpha t}) \\ \frac{1}{2} \frac{\partial^3 f}{\partial x \partial y^2} = 2 \left(M - \frac{M-1}{\bar{v}} \right)^2 ((M-1) D_2)^2 \left[\left((\alpha t)^2 - \alpha t - \frac{3}{2} \right) e^{-\alpha t} + 4\alpha t e^{-2\alpha t} + \frac{3}{2} e^{-3\alpha t} \right] \\ \quad + \frac{3}{2} \left(M - \frac{M-1}{\bar{v}} \right)^2 (M-1) D_3 ((2\alpha t - 3) e^{-\alpha t} + 4e^{-2\alpha t} - e^{-3\alpha t}) \end{array} \right. \quad (28)$$

Fig. 5 shows the simulation results in red along with the moments given by Eqs. 28 in green.

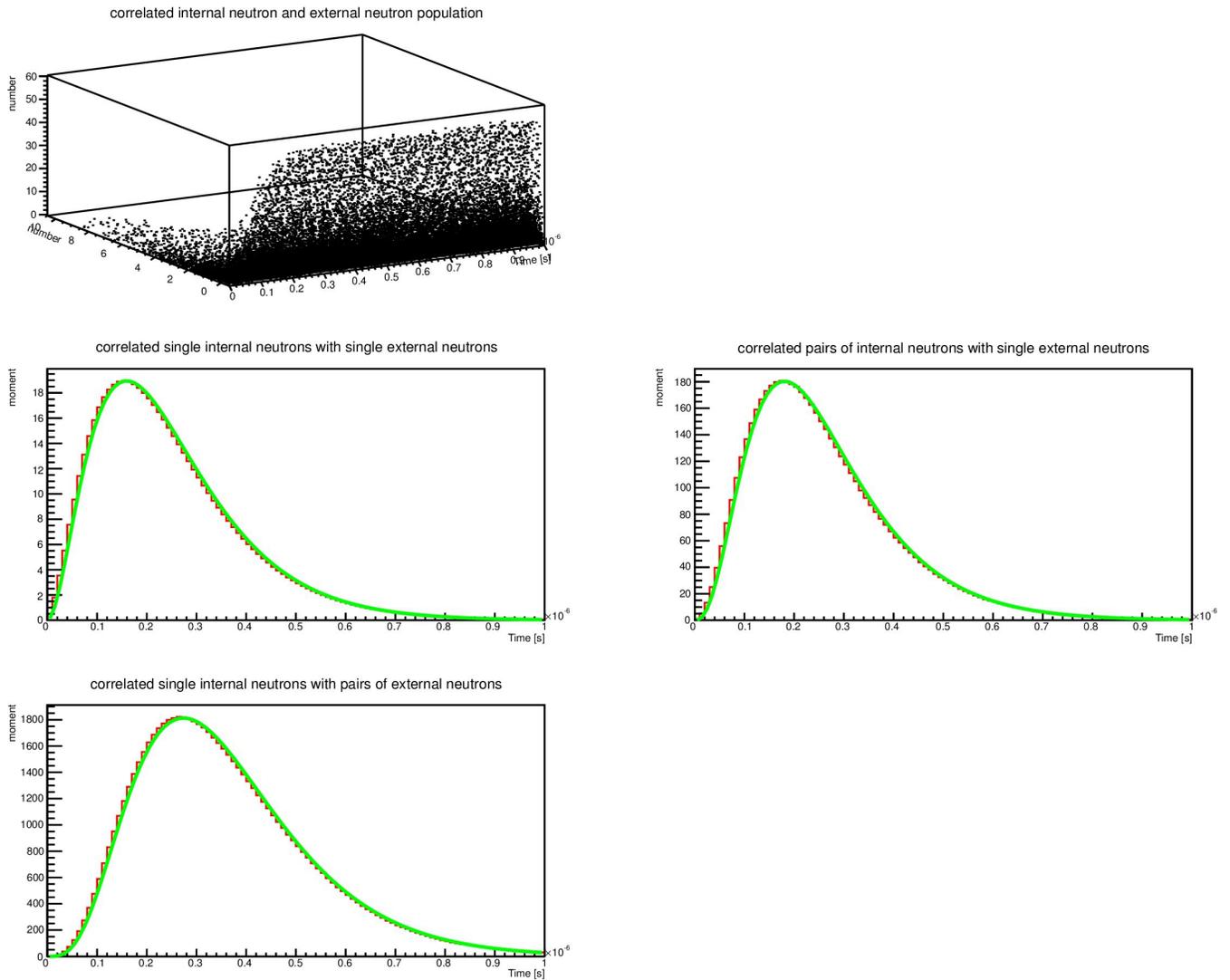


Figure 5: Time evolution of the correlated internal neutron population and external neutron population. The Monte-Carlo simulation was a random source emitting single neutrons, the multiplying isotope was ^{235}U of multiplication 10. The nuclear data for the induced fission of ^{235}U were evaluated at 1 MeV. $\tau=10$ ns, source strength=1000 neutrons/sec, data time=12 hours.

The moments of the correlated external neutron and fission populations are

$$\left\{ \begin{aligned}
 \frac{\partial^2 f}{\partial y \partial z} &= 2qM \left(\frac{M-1}{\bar{v}} \right)^2 v_2 (1 - 2\alpha t e^{-\alpha t} - e^{-2\alpha t}) + qM(M-1) (1 - e^{-\alpha t} - \alpha t e^{-\alpha t}) \\
 \frac{1}{2} \frac{\partial^3 f}{\partial y^2 \partial z} &= 3(qM)^2 \left(\frac{M-1}{\bar{v}} \right)^3 v_2^2 \left((1 - 2\alpha t - 2(\alpha t)^2) e^{-\alpha t} - (4\alpha t + 2) e^{-2\alpha t} + 2 - e^{-3\alpha t} \right) \\
 &+ (qM)^2 \left(\frac{M-1}{\bar{v}} \right)^2 v_2 \bar{v} \left(3 - (2(\alpha t)^2 + 4\alpha t) e^{-\alpha t} - (2\alpha t + 3) e^{-2\alpha t} \right) \\
 &+ \frac{3}{2} (qM)^2 \left(\frac{M-1}{\bar{v}} \right)^2 v_3 \left((3 - 6\alpha t) e^{-\alpha t} - 6e^{-2\alpha t} + e^{-3\alpha t} + 2 \right) \\
 &+ (qM)^2 \frac{M-1}{\bar{v}} v_2 (1 - 2\alpha t e^{-\alpha t} - e^{-2\alpha t}) \\
 \frac{1}{2} \frac{\partial^3 f}{\partial y \partial z^2} &= -6qM \left(\frac{M-1}{\bar{v}} \right)^2 \left(\frac{M-1}{\bar{v}} v_2 \right)^2 \left(\frac{1}{2} e^{-3\alpha t} + (1 + 2\alpha t) e^{-2\alpha t} + \left((\alpha t)^2 + \alpha t - \frac{1}{2} \right) e^{-\alpha t} - 1 \right) \\
 &+ 3qM \left(\frac{M-1}{\bar{v}} \right)^2 \frac{M-1}{\bar{v}} v_3 \left(\frac{1}{2} e^{-3\alpha t} - 3e^{-2\alpha t} - \left(3\alpha t - \frac{3}{2} \right) e^{-\alpha t} + 1 \right) \\
 &- 2qM \left(\frac{M-1}{\bar{v}} \right)^3 \bar{v} v_2 \left((2\alpha t + 3) e^{-2\alpha t} + (2(\alpha t)^2 + 4\alpha t) e^{-\alpha t} - 3 \right) \\
 &- 2qM \left(\frac{M-1}{\bar{v}} \right)^2 v_2 (e^{-2\alpha t} + 2\alpha t e^{-\alpha t} - 1) \\
 &- qM \left(\frac{M-1}{\bar{v}} \right)^2 \bar{v}^2 \left(\left(\frac{1}{2} (\alpha t)^2 + \alpha t + 1 \right) e^{-\alpha t} - 1 \right)
 \end{aligned} \right. \tag{29}$$

Fig. 6 shows the simulation results in red along with the moments given by Eqs. 29 in green. One should point out that due to what appears to be computer memory limitations, the multiplication was not set to 10 in this case, but to 5.

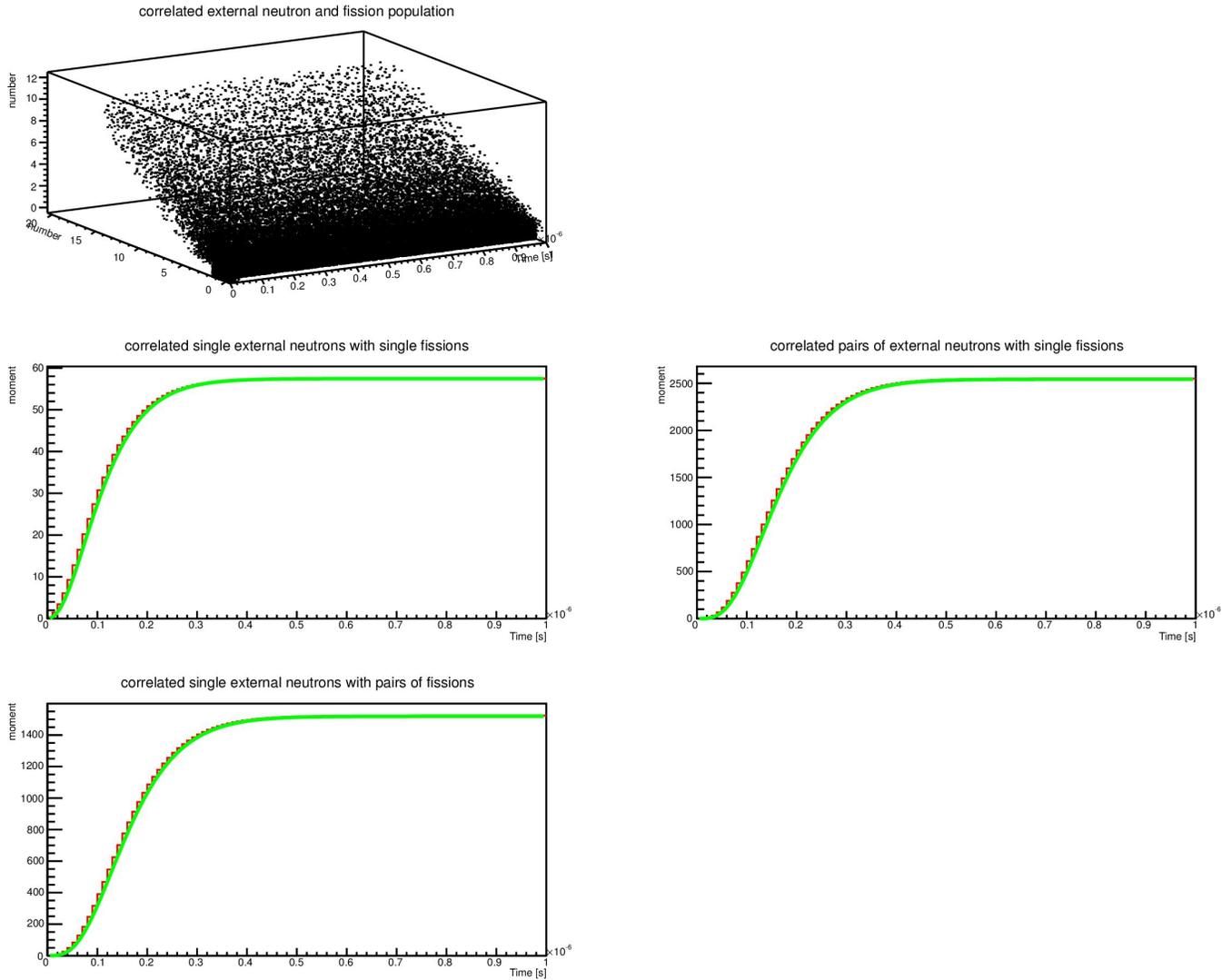


Figure 6: Time evolution of the correlated external neutron population and fission population. The Monte-Carlo simulation was a random source emitting single neutrons, the multiplying isotope was ^{235}U of multiplication 5. The nuclear data for the induced fission of ^{235}U were evaluated at 1 MeV. $\tau=10$ ns, source strength=1000 neutrons/sec, data time=12 hours.

7 Conclusion

Starting from the rate equation describing the time evolution of neutron populations, we developed an algorithm to simulate fission chains. The algorithm correctly reproduced the moments of three different populations taken individually: the internal neutron population, the external neutron population, and the fission population; as well as moments of two correlated populations.

A Internal neutron population

Ref. [2] lists the differential equations for the populations of internal neutrons, external neutrons, and fissions. These differential equations were solved numerically with two independent codes: Mathematica [3] and a solver due to one of the co-authors M. Prasad. In the next 3 sections, the numerical solutions due to M. Prasad are shown in red against the solutions obtained by Monte-Carlo in blue.

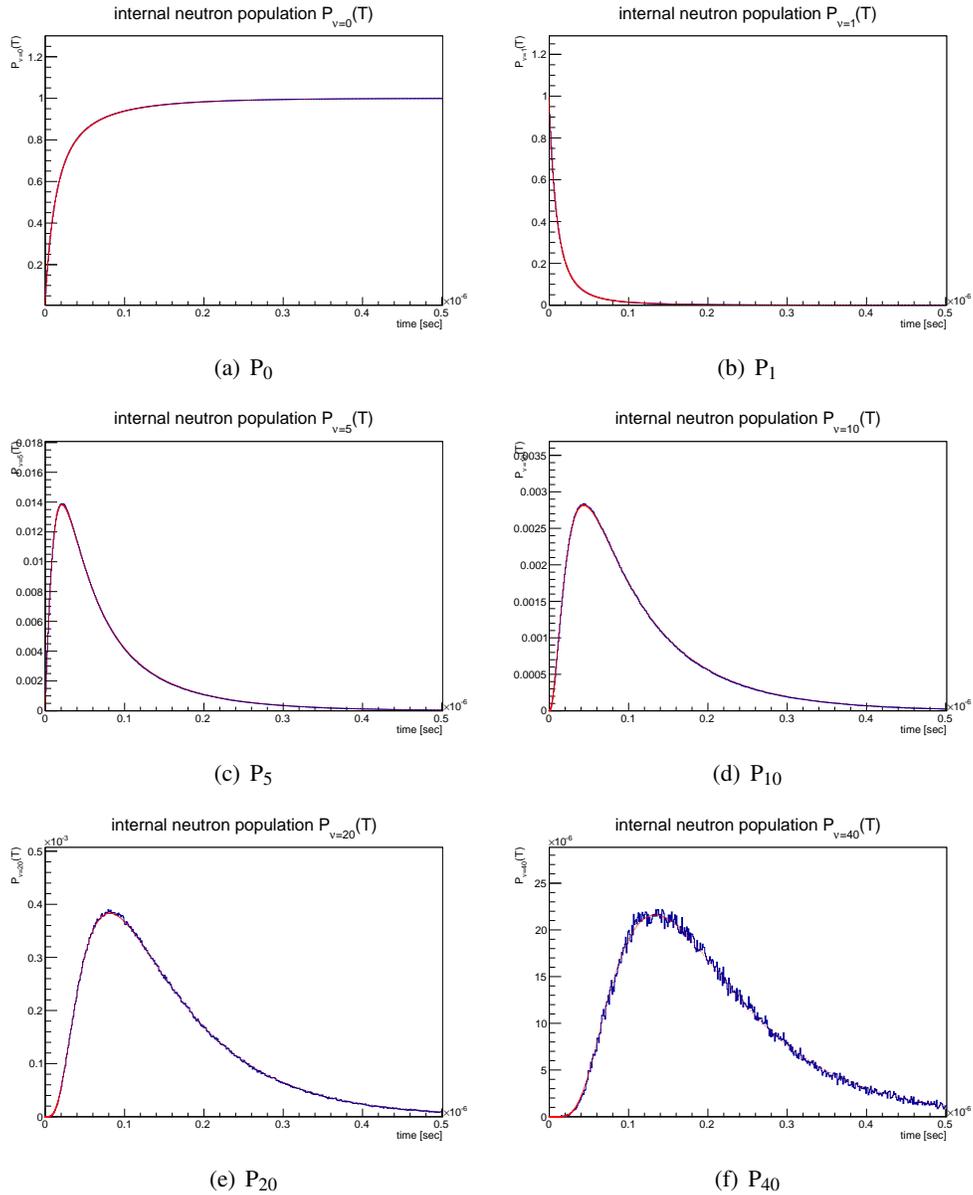


Figure 7: Distribution P_v of internal neutrons. The Monte-Carlo simulation (blue) was a random source emitting single neutrons, the multiplying isotope was ^{235}U of multiplication 10. The nuclear data for the induced fission of ^{235}U were evaluated at 1 MeV. $\tau=10$ ns, source strength=1000 neutrons/sec, data time=12 hours. In red, M. Prasad's numerical solution to differential equation in Ref. [2].

B External neutron population

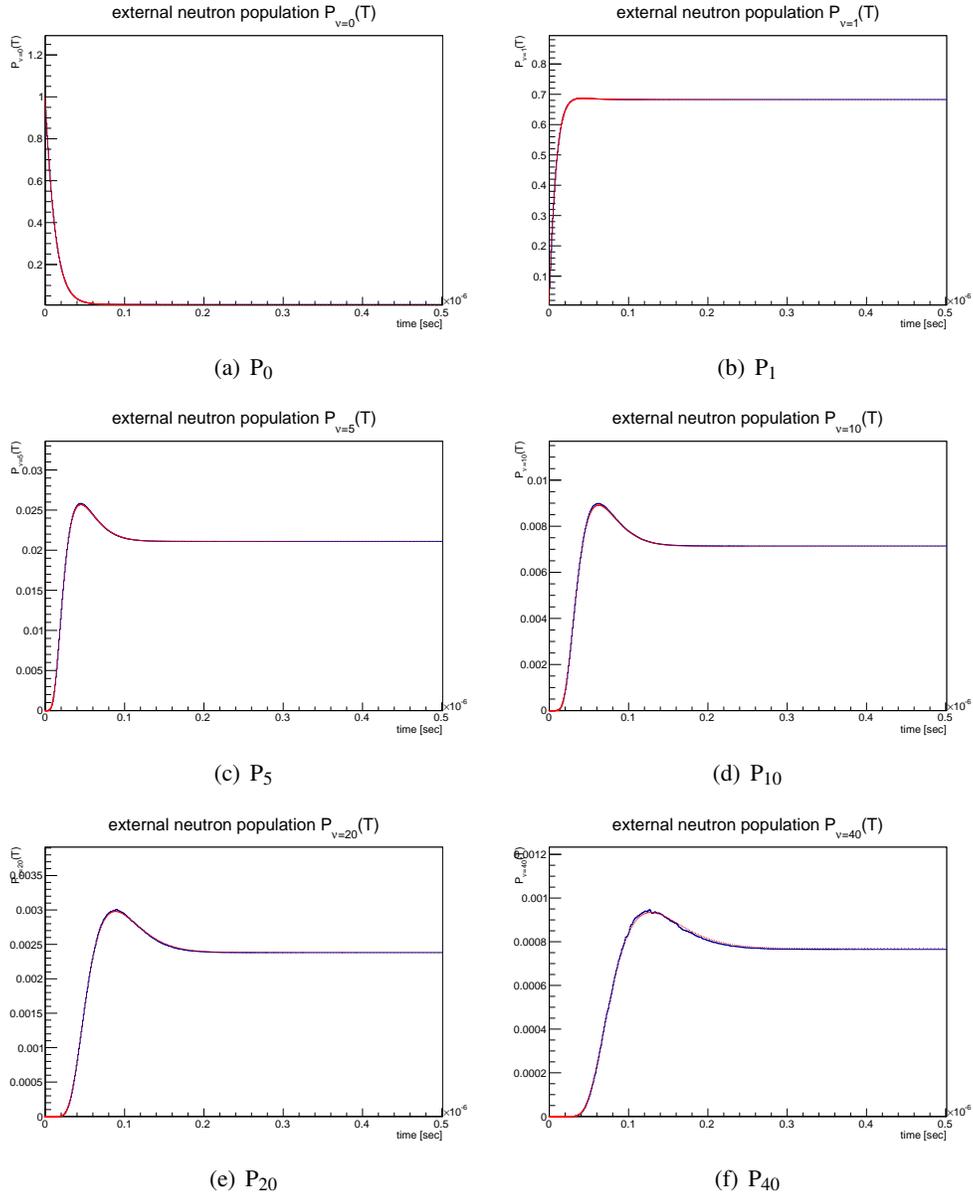


Figure 8: Distribution P_v of external neutrons. The Monte-Carlo simulation (blue) was a random source emitting single neutrons, the multiplying isotope was ^{235}U of multiplication 10. The nuclear data for the induced fission of ^{235}U were evaluated at 1 MeV. $\tau=10$ ns, source strength=1000 neutrons/sec, data time=12 hours. In red, M. Prasad's numerical solution to differential equation in Ref. [2].

C Fission population

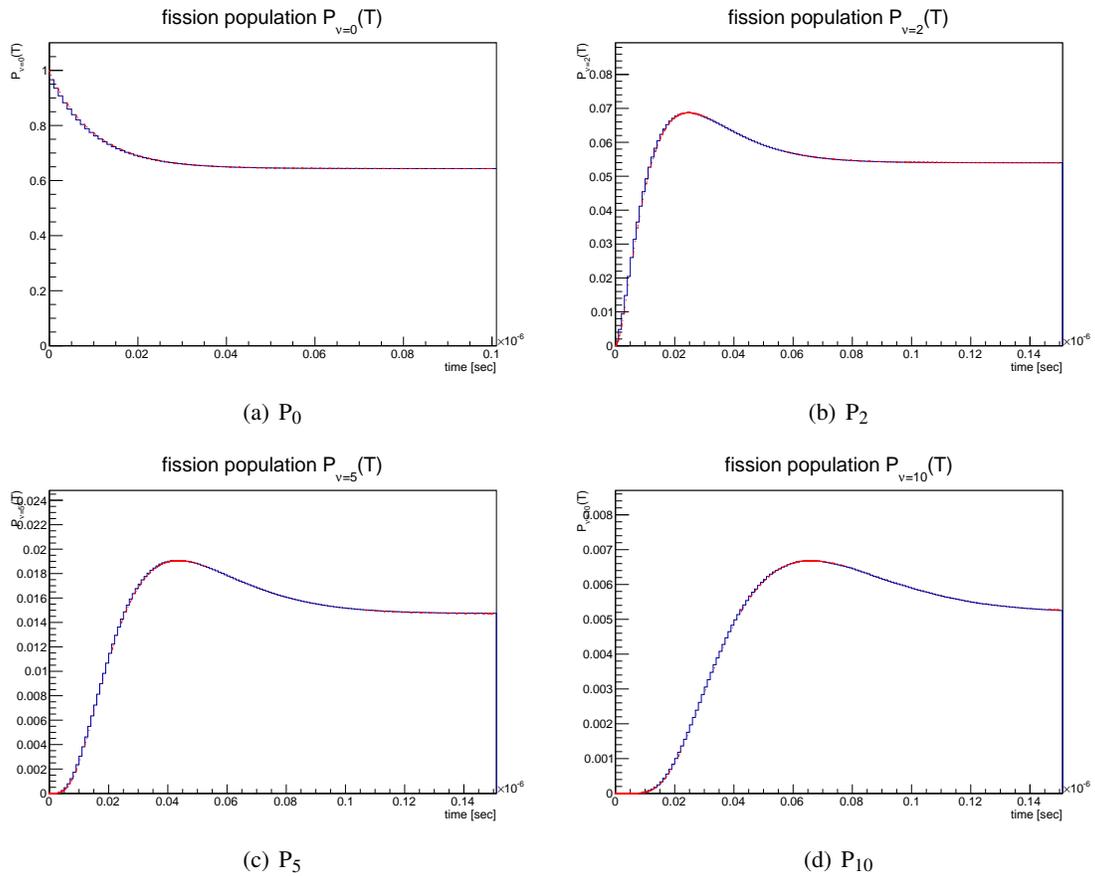


Figure 9: Distribution P_v of number of fissions. The Monte-Carlo simulation was a random source emitting single neutrons, the multiplying isotope was ^{235}U of multiplication 10. The nuclear data for the induced fission of ^{235}U were evaluated at 1 MeV. $\tau=10$ ns, source strength=1000 neutrons/sec, data time=12 hours. In red, Mathematica's [3] numerical solution to differential equation in Ref. [2].

References

- [1] J.M. Verbeke, “Snyderman-Prasad lectures on Fission Chains,” LLNL-TR-, Lawrence Livermore National Laboratory (2013). [1](#)
- [2] K.S. Kim, L. Nakae, N.J. Snyderman, M.K. Prasad, J.M. Verbeke, “Time evolving fission chains and fast neutron and γ -ray counting,” *to be submitted to a journal*, Lawrence Livermore National Laboratory (2013). [7](#), [17](#), [18](#), [19](#)
- [3] Wolfram Research, Inc., Mathematica, Version 8.0, Champaign, IL (2010). [17](#), [19](#)