#### Monte Carlo Calculation of Moments of the Neutron Number and Fission Number for Stochastic Systems in MCATK

Travis J. Trahan

Los Alamos National Laboratory, PO Box 1663, Los Alamos, NM, 87545, tjtrahan@lanl.gov

**Abstract** – Stochastic systems are those in which the observed behavior of the system may differ greatly from the expected or average behavior of the system. Typically this occurs in systems with low neutron populations where the random behavior of the individual neutrons is observable in the systems' aggregate behavior. These systems cannot be characterized by their mean behavior alone. In this paper, a Monte Carlo method for calculating statistical moments of the neutron number and fission number for stochastic systems is presented. This method has been implemented in the Monte Carlo Application ToolKit (MCATK), which is used to generate results for two numerical test problems. The results presented in this paper indicate that the Monte Carlo method provides a viable alternative to deterministic methods for calculating these statistical moments.

## I. INTRODUCTION

Typical nuclear engineering applications are concerned with systems in which the neutron population is large. In such a system there are so many neutrons that fission chains overlap, and the average behavior of the neutrons is sufficient to describe the system. Systems that are well characterized by their mean behavior may be referred to as deterministic.

However, in systems with weak neutron sources, i.e., small neutron populations, the fission chains do not overlap, and the random behavior of the individual neutrons and fission chains is observable in the systems' aggregate behavior. For example, even in a static system, the total neutron population may vary wildly as individual fission chains grow or die away. In criticality accidents with weak sources, it is possible that all fission chains terminate, resulting in no harm done, or that some small number of them diverge, causing possible harm to exposed workers. One must therefore characterize the distribution of possible stochastic system states using more than just the average state in order to fully understand criticality accident scenarios. Analysis of neutron noise in stochastic systems is also important for nuclear material characterization in safeguards applications.

Deterministic equations for characterizing stochastic systems were first developed by Bell [1]. These coupled equations take the form of adjoint transport equations with modified source terms. Deterministic analysis of stochastic systems has been implemented in PARTISN [2] and PANDA [3].

Since the systems being considered are stochastic, it is quite natural to apply the Monte Carlo method to characterize their behavior. Because the individual fission chains do not overlap and must be considered as independent entities, we must follow individual fission chains and observe their stochastic behavior.

For example, if one wanted to calculate the risk of a specific criticality excursion, one could tally for every fission chain the dose at a particular location. If this is done

for enough chains, one may form a distribution of doses that could be observed during an accident and estimate the probability that a particular criticality excursion results in a dose exceeding a certain level. Another way to characterize a stochastic system is to create a distribution of the number of neutrons alive in the system at a particular instant in time (referred to here as the "neutron number"), or a distribution of the total number of fissions that have occurred up to an instant in time (referred to here as the "fission number"). These distributions may be characterized by their moments.

Other quantities of interest that may be obtained via fission chain analysis are: (1) system multiplication – the expected number of progeny produced for each source particle, (2) probability of initiation (POI) – the probability of a fission chain persisting for an infinite period of time, and (3) probability of survival (POS) – the probability of a fission chain persisting, or surviving, until a designated end time. Monte Carlo POI capabilities have been implemented in the Mercury code [4,5,6], a research version of the MCNP code [7], and the Monte Carlo Application ToolKit (MCATK) [8]. Monte Carlo POS capabilities for dynamic systems have also been implemented in MCATK [9]. MCATK is a component-based toolkit developed at Los Alamos National Laboratory and designed to enable rapid development of specialized Monte Carlo applications [10].

In this work, we show how moments of the neutron and fission number distributions can be calculated by direct forward Monte Carlo simulation. This method has been implemented in MCATK.

In the following sections, we review the dynamic fission chain analysis algorithm implemented in MCATK. We then show how this capability can be extended to calculate the moments of the neutron and fission number distributions for single fission chains. Next, we show how formulas describing compound Poisson distributions can be applied to combine source rate information with the single chain moments to obtain moments that account for the presence of multiple fission chains. The methodology is applied to two simple systems, and Monte Carlo results are compared to deterministic calculations. We conclude with a

brief summary of the work and discussion of proposed future work.

## II. DYNAMIC FISSION CHAIN ANALYSIS ALGORITHM IN MCATK

An algorithm for fission chain analysis of dynamic, stochastic systems has been implemented in MCATK [9]. The fission chain algorithm requires that each source particle receive a unique ID number. All progeny of that source particle are given the same ID number, allowing each to be identified as a member of a unique fission chain. With this information, the population of a chain at any given time is known, and virtually any standard tally can be accumulated on a chain by chain basis based on the ID of the particle being tallied. In this work, we will tally the neutron number and fission number for every chain at specified points in time.

In a dynamic system, every fission chain must be followed through the evolving system until its death or the end of simulation. If the chains are allowed to grow in an analog fashion, divergent chains may reach a population that exceeds memory limitations on a given computer. Population control is used in MCATK simulations of deterministic systems to limit maximum size of the Monte Carlo particle population for supercritical systems, or to prevent the Monte Carlo particle population from vanishing for subcritical systems [11]. We have applied the population control method to the fission chain algorithm.

In supercritical stochastic systems, some chains may diverge but many will die out naturally. Since the death of a fission chain is something we are interested in observing, it is undesirable to keep the chain alive via population control. Thus, we cannot apply population control to the entire Monte Carlo particle population. Instead, we must allow the chains to behave stochastically until the instantaneous chain population exceeds a threshold, at which point we consider that chain "deterministic". Each chain will be considered stochastic or deterministic on an individual basis.

Once a chain becomes deterministic, the standard population control used in MCATK is applied to that chain, but not to the overall Monte Carlo particle population. The population control is only applied at the end of a time step. Each chain begins with a weight equal to the weight of the initiating particle. Nominally, every particle in the chain will have this same weight. When population control is applied to a chain, the individual particle weights vary. The chain weight is set to the target average particle weight, that is, the desired weight of particles surviving population control in order to preserve the pre-population control weight of the chain.

Typical criticality excursions may be supercritical for a time, but then enter a subcritical state. At this point, chains that had diverged will begin to shrink. As the population shrinks, splitting will be applied and the chain and particle weights will be reduced. If the splitting process were allowed to continue indefinitely, the once-divergent chains would never die. To avoid this undesirable behavior, when the chain weight drops below its original starting weight due to repeated splitting, the chain is once again considered stochastic, and the population control is turned off.

MCATK has the ability to load balance parallel runs by shifting particles from one process to another. In fission chain analysis mode, the communication required to identify all particles in the same fission chain is thought to be prohibitive. Thus, chains are kept entirely on one process. This restriction can lead to load imbalance, resulting in decreased performance and possibly code failure due to some processors exceeding memory limitations. To avoid exceeding memory limits in this mode, one may have to use more processors than would be required if load balancing were used, or else use more aggressive population control.

Source time biasing has been implemented in MCATK. Fission chains that originate near first criticality (the time in an accident scenario in which the system first becomes supercritical) will have the longest opportunity to grow. Therefore, these chains are the most important, and it can be helpful to bias the source towards times near first critical.

Spontaneous fission sources in MCATK are typically modeled by emitting exactly one fission neutron per source event, and multiplicity is accounted for by increased the source rate. Thus, there is no correlation accounting for multiple neutrons emitted from a single fission. MCATK now includes the ability to sample from multiplicity data (data obtained from [12]) for various isotopes in order to create between 0 and 9 neutrons per source event. In the fission chain analysis mode, all of these neutrons are treated as part of the same fission chain. Source neutrons emitted from the same event are correlated in space and time, but their energies and angles are still sampled independently. Thus, the multiplicity treatment is only approximate.

#### **III. CALCULATING MOMENTS OF THE NEUTRON AND FISSION NUMBER DISTRIBUTIONS**

In this section, we derive a Monte Carlo method for calculating the moments of the neutron and fission number distributions. The moments are tallied for individual fission chains, and then this information is used in conjunction with source information to obtain moments for the full system, which contains a random number of fission chains. Tallying the moments requires identifying which particles belong to each unique fission chain, as described in Section II.

## **1.** Calculation of Moments of the Neutron and Fission Number Distributions for Individual Fission Chains

Each fission chain is independent of all other fission chains, and therefore serves as an independent sample of the neutron and fission numbers for a single fission chain. Let the independently and identically distributed (IID) variable Y represent the distribution of the desired quantity, either

neutron or fission number. Let the neutron or fission number of a single chain *i* be  $y_i$ , and the weight of that fission chain be  $w_i$ . Then the first four zero-based moments of that distribution (i.e., moments about zero, rather than about the sample mean) are given by:

$$E[\mathbf{Y}] = \sum_{i} w_{i} y_{i} / \sum_{i} w_{i}, \qquad (1)$$
$$E[\mathbf{Y}^{2}] = \sum_{i} w_{i} y_{i}^{2} / \sum_{i} w_{i}, \qquad (2)$$
$$E[\mathbf{Y}^{3}] = \sum_{i} w_{i} y_{i}^{3} / \sum_{i} w_{i}, \qquad (3)$$
$$E[\mathbf{Y}^{4}] = \sum_{i} w_{i} y_{i}^{4} / \sum_{i} w_{i}. \qquad (4)$$

MCATK computes these four moments at the end of every time step in dynamic simulations. Fission chains that have died, i.e., no longer have any living neutrons, score a 0 to the neutron number, but may still score a non-zero fission number because that quantity is the number of fissions observed up to that point in time.

## **2.** Calculation of Moments of the Neutron and Fission Number Distributions for a Specified Source Rate

Once zero-based moments of neutron and fission number are known for an individual chain, we must account for the fact that the number of fission chains in the system is random and dependent on the expected source rate. Let the distribution X represent the total neutron and fission numbers for the system at a given time. This distribution is a sum of distributions for individual fission chains over all the fission chains actually in the system:

$$\mathbf{X} = \sum_{i=1}^{N} Y_i, \tag{5}$$

where *N* is itself a random variable representing the number of fission chains. Spontaneous fission is a Poisson process, and so *N* is described by a Poisson distribution. The Poisson distribution has a single parameter,  $\lambda$ , which is the expected number of events within a designated interval. Therefore,  $\lambda$ is the source rate (neutrons per second or fissions per second depending on if spontaneous fission multiplicities are used) multiplied by time elapsed between the start of the problem and the current time step. By convention, if *N*=0, the sum in Eq. (5) is 0.

In general, distributions given by a random sum of random variables, as in Eq. (5), are referred to as *compound distributions*. When the variable N is defined by a Poisson distribution, as is the case in radioactive decay, the distribution is a compound Poisson distribution. Compound Poisson distributions appear frequently in actuarial mathematics. For example, the IID Y could represent the

cost of a single insurance claim, while the number of claims observed would be given by the IID N, which is also described by a Poisson distribution. Thus, the mean, variance, skewness, and kurtosis of the compound Poisson distribution are well known, and are given by [13,14]:

$$\mathbf{E}[\mathbf{X}] = \lambda E[Y],\tag{6}$$

$$\sigma^2(X) = \lambda E[Y^2],\tag{7}$$

$$\operatorname{Skew}(X) = \lambda E[Y^3] / \sigma^3(X), \quad (8)$$

$$\operatorname{Kurt}(X) = \lambda E[Y^4] / \sigma^4(X). \tag{9}$$

We see that the moments of the total neutron or fission numbers can be calculated using only the expected number of fission chains initiated in the time interval and the zerobased moments of the neutron or fission number for single chains given by Eqs. (1)-(4). As one would expect, the expected neutron or fission number is simply the expected number for a single chain multiplied by the expected number of chains. Perhaps most interestingly, we observe that as the source rate (i.e.,  $\lambda$ ) increases, the skewness and kurtosis decrease, and the mean increases faster than the standard deviation. In other words, as the source rate increases, the neutron and fission numbers become first normal, and then approach a delta function. This confirms the idea that systems with strong sources behave deterministically, being sufficiently characterized by only their mean behavior, while systems with weak sources behave stochastically and must be characterized by additional statistical moments.

## **IV. RESULTS**

We now demonstrate the Monte Carlo calculation of moments of the neutron and fission number distributions as described in Section III. The moment tallies were implemented in MCATK, and are applied to two example problems. The MCATK moment tally results are compared to PARTISN results gathered from other sources.

Neither test problem makes use of the spontaneous fission source multiplicity capability in MCATK. There are two reasons for this. First, an equivalent deterministic capability is not implemented in PARTISN at this time. Second, preliminary results indicated that the effect on the moments was not significant. The results did suggest that fewer chains exist at any given time with only one or two neutrons, as would be expected since not every chain is born with exactly one neutron. However, the effect on the moments of the neutron and fission numbers, if any, was smaller than the statistical uncertainty of those moments.

## 1. Static Test Problem: Plutonium Sphere

We consider a 6.5 cm sphere of enriched plutonium (95.5 wt% Pu-239 and 4.5 wt% Pu-240) with density 15.66

g/cc. The total source rate is  $0.847254 \text{ n/}\mu\text{s}$ . For simplicity, all source neutrons are sampled using Pu-240 data. The dominant source of spontaneous fission is Pu-240, with roughly 0.03% coming from Pu-239. Therefore, using only Pu-240 neutrons is expected to have negligible effect.

Dynamic simulations are performed for 0.5  $\mu$ s, and the moments of the neutron and fission number distributions are calculated at this final time. Thirty independent calculations are performed with 38.4 million Monte Carlo fission chains per calculation (7.5E4 fission chains for each of 512 parallel processes in each calculation). Fission chains are initiated with one source particle, i.e., without sampling spontaneous fission multiplicity data. Time biasing is used such that 20% of the fission chains are born in each of 5 time intervals: [0.00, 0.01, 0.03, 0.10, 0.20, 0.50]  $\mu$ s. The mean and standard deviation of the first four zero-based moments of the neutron and fission numbers are calculated using the thirty independent samples of these quantities (see Table I).

Table I. Mean and Standard Deviation of Zero-Based Moments of Single Fission Chain Neutron and Fission Number for Pu Test Problem.

	Neutron Number Mean Relative Std. Dev.		Fission Number	
			Mean	Relative Std. Dev.
E[Y]	1.389e1	1.924e-3	1.454e2	1.698e-3
$E[Y^2]$	5.945e4	3.221e-3	6.133e6	3.315e-3
$E[Y^3]$	5.206e8	6.977e-3	5.476e11	7.542e-3
$E[Y^4]$	6.922e12	1.557e-2	7.432e16	1.629e-2

Table II. Comparison of MCATK and PARTISN Neutron Number Distribution Parameters for Pu Test Problem.

	MCATK	PARTISN	Rel. Diff.
Mean	5.884e0	6.055e0	-2.824e-2
Std. Dev.	1.587e2	1.620e2	-2.057e-2
Skewness	5.519e1	5.480e1	7.049e-3
Kurtosis	4.624e3	4.569e3	1.204e-2

Table III. Comparison of MCATK and PARTISN Fission Number Distribution Parameters for Pu Test Problem.

	MCATK	PARTISN	Rel. Diff.
Mean	6.158e1	6.301e1	-2.268e-2
Std. Dev.	1.612e3	1.638e3	-1.582e-2
Skewness	5.539e1	5.501e1	6.938e-3
Kurtosis	4.664e3	4.609e3	1.194e-2

Given the source rate of 0.847254 neutrons/ $\mu$ s and simulation time of 0.5  $\mu$ s, we find that the Poisson parameter  $\lambda$  (i.e., the expected number of fission chains) is 0.423627. Introducing the zero-based single fission chain moments from Table I into Eqs. (6)-(9) gives us the first four statistical moments of the neutron and fission number distributions for the system (see Tables II and III).

The ability to calculate the moments of the neutron and fission number distributions has also been implemented in the  $S_N$  code PARTISN [15]. PARTISN results for this problem, provided by E. Fichtl of Los Alamos National Laboratory, are also shown in Tables II and III.

We see that the differences between the codes is roughly 1-3%, which for the mean and standard deviation is outside the statistical uncertainty of those quantities. Still these errors are reasonable considering the differences between the methods used to calculate the moments. PARTISN uses the S<sub>N</sub> method to solve a series of related adjoint transport equations with non-standard source terms. The four adjoint equations for the first four moments must be solved sequentially, and a separate calculation must be performed to calculate the moments for every desired point in time. By comparison, the Monte Carlo method performs a single, standard forward calculation with non-standard tallies, and while keeping track of which fission chain each particle belongs to. The single calculation yields the moment at every time step. The Monte Carlo method also does not require approximate angular treatments, and, perhaps most significantly, uses continuous energy, rather than multigroup, cross section data. Given these differences between the methodologies, the agreement between the two codes is acceptable.

# 2. Dynamic Test Problem: Uranium Sphere with Changing Enrichment

Next, we consider a benchmark criticality excursion first proposed by Baker [16] and again studied by Fichtl [15]. The system is a 17.25 cm sphere of a time-varying mixture of uranium-235 and uranium-238. The total density of the sphere is a constant 15 g/cc. The densities of the two uranium isotopes versus time are given in Table IV. The isotopic compositions vary linearly between the times shown in Table IV, but are only updated at the end of each 1 sh time step. We note that unit of time shake [sh] used throughout this section is equivalent to 1e-8 sec. The system first reaches criticality at 200 sh, is at its maximum criticality from 400 to 500 sh, and returns to a subcritical state at 700 sh.

Table IV. Isotopic Densities for the U Test Problem

FIODIeIII.		
Time	U235 Density	U238 Density
[sh]	[g/cm <sup>3</sup> ]	$[g/cm^3]$
0	5.0	10.0
200	6.5	8.5
400	14.0	1.0
500	14.0	1.0
700	6.5	8.5
900	5.0	10.0
1000	5.0	10.0

The source used in the MCATK calculations is monoenergetic and uniformly distributed in space. The source energy, 14.1627 MeV, was chosen to be consistent with energy group 7 of the 133 group MENDF6 multigroup cross section set. Unfortunately, the anticipated PARTISN calculations at this source energy have not yet been completed. Instead, we will compare the MCATK calculations to the original PARTISN calculations [15], which used a uniformly distributed source in space and energy (i.e., every energy group had an identical source rate). Time biasing was used in order to increase the number of fission chains born around the time of first criticality. The biased number of fission chains per time step as a function of time is given in Table V. The total number of fission chains per calculation is 182400.

Table V. Monte Carlo Fission Chain Sampling Rates versus Time for the U Test Problem

Rates versus	Time for the U	Test Problem.
Start	Stop	Chains Per
[sh]	[sh]	Shake
0	150	64
150	300	512
300	500	256
500	700	128
700	1000	64

Forty calculations were performed with a combing threshold of 1000. Another thirty-four have been run so far with a combing threshold of 10000. The lower threshold runs are performed using 64 processors per calculation, and take approximately 3.5-4.0 hours to complete. The higher threshold runs are performed using with varying numbers of processors. In all cases, calculations are run "undersubscribed", meaning that fewer than the maximum number of processors are used per compute node in order to increase the memory available per process. Several calculations used 16 nodes each, with 16 processors out of 36 per node, and each took between 6.75-7.25 hours to complete.

Each calculation for a given threshold serves as an independent sample of the moments, which enables the calculation of their mean and relative error. The mean and relative error of the neutron and fission moments at first and second criticality are presented in tables VI and VII.

The first moment of both the neutron and fission number distributions is relatively unaffected by the value of the combing threshold. However, the higher moments are greatly affected, with the kurtosis changing by over two orders of magnitude at second criticality (out of roughly 220 orders of magnitude). Increasing the population control threshold decreases the relative standard deviation of the moments significantly at second criticality. The effect of the threshold on the mean values indicates that the moment tallies are not fully converged with a threshold of only 1000 particles. This is because with only 1000 particles per chain,

Table VI. Mean and Standard Deviation of Zero-Based
Moments of Single Fission Chain Neutron Number for the
U Test Problem.

	First Critical (Time = $200 \text{ sh}$ )				
	Population Control Threshold = 1e3		Population Control Threshold = 1e4		
	Mean Relative Std. Dev.		Mean	Relative Std. Dev.	
E[Y]	0.799e-1	0.06564	7.868e-1	0.06695	
$E[Y^2]$	4.749e1	0.17034	4.701e1	0.16947	
$E[Y^3]$	5.436e3	0.32028	5.480e3	0.32300	
$E[Y^4]$	8.722e5	0.49970	8.999e5	0.51465	
	Sec	ond Critical	(Time = 700)	sh)	
	$\frac{Population Control}{Threshold = 1e3}$ $\frac{Mean}{Std. Dev.}$		Population Control Threshold = 1e4		
			Mean	Relative Std. Dev.	
E[Y]	1.202e52	0.12213	1.201e52	0.05841	
$E[Y^2]$	1.493e107	0.83677	4.600e106	0.13961	
$E[Y^3]$	8.985e162	2.07834	3.634e161	0.26397	

Table VII. Mean and Standard Deviation of Zero-Based Moments of Single Fission Chain Fission Number for the U Test Problem.

	First Critical (Time = $200 \text{ sh}$ )			
	Population Control Threshold = 1e3		Population Control Threshold = 1e4	
	Mean Relative Std. Dev.		Mean	Relative Std. Dev.
E[Y]	1.332e1	0.04549	1.321e1	0.04510
$E[Y^2]$	4.767e3	0.16629	4.593e3	0.16530
$E[Y^3]$	4.619e6	0.34160	4.331e6	0.33283
$E[Y^4]$	6.844e9	0.56660	6.283e9	0.56083
	Sec	ond Critical	(Time = 700)	sh)
	$\begin{tabular}{lllllllllllllllllllllllllllllllllll$		Population Control Threshold = 1e4	
			Mean	Relative Std. Dev.
E[Y]	8.660e52	0.12232	8.647e52	0.05763
$E[Y^2]$	7.572e108	0.92997	2.377e108	0.13771
$E[Y^3]$	3.325e165	2.29824	1.347e164	0.26723
$E[Y^4]$	3.284e222 3.52879		1.175e220	0.56840

and with chains achieving such large weights, random, large fluctuations in the total weight of the chain can occur. Using 10000 particles per chain is certainly better, but the population control threshold should be increased further to verify that the tallies have converged with respect to the combing threshold. This will be left for future work. Although the errors may seem large at first glance, they are quite small when one considers that the neutron population grows 53 orders of magnitude between first and second criticality, and that the largest moments exceed  $10^{220}$ .

Figures 1 and 2 show the neutron and fission number moments as a function of time for a source rate of 0.01 n/sh. The combing threshold for these results was 10000. True



(b) PARTISN. Figure reproduced from Ref. 15, Fig. 3.

Fig 1. Natural log of the moments of the neutron number distribution for the uranium sphere test problem. The MCATK plot depicts, for each moment, calculations with the highest and lowest peak values (lighter, thinner lines), as well as the average over all calculations (darker, thicker lines). error bars for these moments cannot be computed at this time. The relative errors of the various zero-based moments are clearly correlated (a high weight chain will score high to all moments), but their covariances are not computed at this time. Therefore, the error in the zero-based moments cannot be propagated to the skewness and kurtosis of the neutron and fission number distributions, as these distributions are calculated using multiple zero-based moments (see Eqs. (8) and (9)). In order to visualize the errors in these moments, we have simply identified the individual calculations with the highest and lowest peak values of the moments, and plotted these alongside the average values of the moments. This gives an approximate bound on the fluctuations in the moments that may be observed.

The natural log of the moments of the neutron number for a source rate of 0.01 n/sh are plotted for MCATK and PARTISN in Figure 1. The PARTISN figure is reproduced from Ref. 15, Figure 3. The codes exhibit good agreement, especially considering that they each used a different source definition. Furthermore, it may be necessary to perform the simulation with a higher population control threshold in order to fully converge the Monte Carlo solution. This is the subject of future work. The high, low, and average MCATK values of each moment are, for the most part, too similar to distinguish.

The natural log of the moments of the fission number for a source rate of 0.01 n/sh are plotted for MCATK in Figure 2. No PARTISN results are available at this time for the fission number moments for this particular problem. The behavior of the fission number moments is similar to the neutron number moments. Again, the high, low, and average values of the moments are too similar to distinguish.



Fig 2. Natural log of the moments of the fission number distribution for the uranium sphere test problem. The plot depicts, for each moment, calculations with the highest and lowest peak values (lighter, thinner lines), as well as the average over all calculations (darker, thicker lines). Combing threshold = 1e4.

Figures 1 and 2 each consider only one source rate: 0.01 n/sh. Next, we consider the effect of changing the source rate. The natural log of the neutron number moments at second criticality (time = 700 sh) are plotted as a function f source strength for both MCATK and PARTISN in Figure 3. The PARTISN figure is reproduced from Ref. 15, Figure 4(a). Again the agreement is good. Only the higher moments, skewness and kurtosis, show any visible differences. The differences can likely be attributed to a combination of different source specifications, and possibly need to increase the population control threshold in the MCATK calculation in order to fully converge the solution.





4(a).

Fig 3. Natural log of the moments of the neutron number distribution at second criticality (time = 700 sh) as a function of source strength.

The behavior of the moments matches the discussion in Section III.2. To reiterate, the skewness and kurtosis decrease as the source rate increases. The standard deviation increases, but the mean increases faster. All this confirms the idea that as the source rate in a system continues to increase, the neutron and fission number distributions become first normal, and then approach a delta function, i.e., the system ceases to be stochastic and becomes deterministic.

The natural log of the fission number moments at second criticality (time = 700 sh) are plotted as a function of source strength for both MCATK and PARTISN in Figure 4. The behavior is the same as for the moments of the neutron number.



Fig 4. Natural log of the moments of the fission number distribution at second criticality (time = 700 sh) as a function of source strength. Combing threshold = 1e4.

#### V. CONCLUSIONS AND FUTURE WORK

In this work, we have presented a novel Monte Carlo algorithm for calculating the moments of the neutron and fission numbers for stochastic systems. Zero-based moments are tallied for individual fission chains, which are tracked by giving all neutrons an ID specifying which chain they belong to. The zero-based moments are then introduced into simple formulas describing compound distributions in order to obtain the mean, variance, skewness, and kurtosis of the neutron and fission numbers accounting for all the fission chains in the system.

Other new features of interest to the fission chain analysis algorithm are: (1) the ability to emit multiple neutrons per spontaneous fission event by sampling from available multiplicity data (results not presented here) and (2) the implementation of source time biasing in order to sample more fission chains with large neutron and fission numbers.

The moments of the neutron and fission number distributions were calculated for two simple test problems using the Monte Carlo method in MCATK and compared to  $S_N$  results from PARTISN. The two codes are in good agreement with one another.

The comparisons of the Monte Carlo and deterministic algorithms for calculating moments of the neutron and fission number distributions yield familiar conclusions. The Monte Carlo algorithm is computationally expensive, and the fission chain algorithm is particularly constrained by memory requirements. However, the Monte Carlo algorithm does have the usual advantages over the deterministic algorithm as well: it uses fewer approximations and does not suffer from discretization errors in space, energy, or angle. The agreement demonstrated here indicates that the Monte Carlo method is a viable alternative to deterministic methods for calculating moments of the neutron and fission number distributions.

The test problems studied here should be re-run using the spontaneous fission multiplicity, in order to better characterize its effect on the tallied moments. If possible, runs with a higher combing threshold should be performed to verify that the moment tallies are converged.

Future work should investigate the effect of load balancing on the fission chain analysis algorithm. The parallel overhead in the code would be increased as fission chains could span multiple processes. However, it would ease restrictions on memory, currently the dominant limitation, by ensuring that large fission chains could not overwhelm some processes while others sit idle. The fission chain analysis algorithm may also be extended to characterize the burst wait time for pulsed reactor experiments.

## ACKNOWLEDGMENTS

The author would like to thank Nicolas Hengartner of Los Alamos National Laboratory for his instruction in compound distributions. The author would also like to thank Erin Fichtl of Los Alamos National Laboratory for motivating this work, serving as a friendly user of these new capabilities in MCATK, and providing PARTISN results.

Los Alamos National Laboratory, an affirmative action/equal opportunity employer, is operated by Los Alamos National Security, LLC, for the National Nuclear Security Administration of the U.S. Department of Energy under contract DE-AC52-06NA25396.

## REFERENCES

1. G. BELL, "On the Stochastic Theory of Neutron Transport," *Nucl. Sci. Eng.*, **21**, 390 (1965).

2. R.E. ALCOUFFE, R.S. BAKER, J.A. DAHL, E.J. FICHTL, S.A. TURNER, R.J. ZERR, "PARTISN: A Time-Dependent, Parallel Neutral Particle Transport Code System," LA-UR-12-23848, Los Alamos National Laboratory (2012).

3. P. HUMBERT, "Stochastic Neutronics with PANDA Deterministic Code," *Proc. M&C* 2003, Gatlinburg, Tennessee, April 7-13, 2003, American Nuclear Society (2003).

4. P.S. BRANTLEY, M.S. MCKINLEY, "Mercury Web Site," Lawrence Livermore National Laboratory, <u>https://mercury.llnl.gov</u>.

5. G. GREENMAN, R. PROCASSINI, C. Clouse, "A Monte Carlo Method for Calculating Initiation Probability," *Proc. M&C+SNA 2007*, Monterey, California, April 15-19, 2007, American Nuclear Society (2007) (CD-ROM).

6. P.S. BRANTLEY, M.S. MCKINLEY, "Probability of Initiation and Extinction in the Mercury Monte Carlo Code," *Proc. M&C 2013*, Sun Valley, Idaho, May 5-9, 2013, American Nuclear Society (2013) (CD-ROM).

7. M.E. RISING, F.B. BROWN, A.K. PRINJA, "The Probability of Initiation in MCNP," *Trans. Am. Nucl. Soc.*, **82**, 134 (2010).

8. S. NOLEN, "Using Fission Chain Analysis to Inform Probability of Extinction/Initiation Calculations with MCATK," *Proc. M&C+SNA+MC* 2015, Nashville, Tennessee, April 19-23, 2015, American Nuclear Society (2015) (CD-ROM).

9. T.J. TRAHAN, S. NOLEN, T. ADAMS, J. SWEEZY, "A Monte Carlo Algorithm for Fission Chain Analysis of Dynamic Stochastic Systems," *Trans. Am. Nucl. Soc.*, **113**, 661 (2015).

10. T. ADAMS, S. NOLEN, J. SWEEZY, A. ZUKAITIS, J. CAMPBELL, T. GOORLEY, S. GREENE, R. AULWES, "Monte Carlo Application ToolKit (MCATK)," *Annals of Nuclear Energy*, **82**, 41 (2015).

11. J. SWEEZY, S. NOLEN, T. ADAMS, A. ZUKAITIS, "A Particle Population Control Method for Dynamic Monte Carlo," *Proc. SNA+MC 2013*, Paris, France, October 27-31, 2013, EDP Sciences - Web of Conferences (2013).

12. J.M. VERBEKE, C. HAGMANN, D. WRIGHT, "Simulation of Neutron and Gamma Ray Emission from Fission and Photofission," UCRL-AR-228518, Lawrence Livermore National Laboratory (2014).

13. P. WLAź, "Approximation of Random Sums of Random Variables in Insurance," *Advances in Science and Technology Research Journal*, **8**(23), 88 (2014).

14. N. HENGARTNER, Personal Communication, December 12, 2015.

15. E.D. FICHTL, R.S. BAKER, "Computing the Moments of the Neutron Population Using Deterministic Neutron Transport," *Proc. M&C 2013*, Sun Valley, Idaho, May 5-9, 2013, American Nuclear Society (2013) (CD-ROM).

16. R.S. BAKER, "Deterministic Methods for Time-Dependent Stochastic Neutron Transport," *Proc. M&C* 2009, Saratoga Springs, New York, May 3-7, 2009, American Nuclear Society (2009) (CD-ROM).