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A Deterministic Transport Method for Calculating the Moments of the Fission Number Distribution

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Abstract - *Fissile systems behave stochastically when the neutron source is weak (e.g. spontaneous fission) because there are not enough neutrons in the system to ensure predictable average behavior. In this case, neutron behavior cannot be fully characterized by an average therefore it is desirable to know the full probability distribution function (PDF) for quantities such as instantaneous neutron number and total fission count. Point ('0-D') and full phase space models that describe the probability distributions of the neutron number have been explored previously, but here we derive a full phase space equation for the moments of the fission number PDF, which is more closely related to radiation dose, and implement these equations in the PARTISN (deterministic transport) code. Numerical results indicate that the neutron and fission number distributions are well-approximated by analytic expressions for the PDF derived using the point model when PARTISN is used to compute the necessary parameters for bare fissile metal spheres.*

I. INTRODUCTION

For many fissile systems, the behavior of the neutron distribution is essentially deterministic, i.e., it is well characterized by its mean, and is therefore predictable. The fission process itself is fundamentally stochastic, however, and deterministic behavior is a fortuitous consequence of individual fission chains overlapping to the extent that they become indistinguishable. In the deterministic limit, it is the mean neutron behavior that drives the evolution of the neutron population. When the source is weak or the neutron population is very small, however, this overlapping cannot occur and stochastic effects become important. It is therefore necessary to treat the inherent stochasticity of the fission process when modeling such systems, which include criticality accident scenarios, passive detection of spontaneous fission sources, reactor startup, criticality excursions in spent fuel etc.

The stochastic neutronics equations that describe the behavior of such systems were first formulated by Bell [1] and Pal [2]. Their equation for the probability generating function of the neutron population distribution is a starting point from which to derive equations for the probability of extinction ($P_{\text{extinction}}$) and its converse, the probability of survival (P_{survival}), the probability of initiation ($P_{\text{initiation}}$), which is the probability that a neutron chain will persist for infinite time, as well as the moments of the neutron population. Another quantity of interest that cannot be directly quantified using this system of equations is the probability of dose, which is related to the number of fissions. Here, we derive a second generating function equation that can be used to generate the moments of the fission number.

Once the moments are known, an additional step is necessary to reconstruct the PDF so that we can, for instance, calculate the probability of exceeding a given dose. In Bell's early work, he was also able to analytically derive a PDF for the neutron number by using a 0-D ('point') model and making a number of simplifying assumptions [3]. In an extension to this work, the authors looked at the joint neutron and fission number distributions for the point model and were able to derive a second analytic PDF for the fission number [4]. Although these PDFs were derived using a low order model, the shape is essentially correct. Here, we explore the use of the full phase-space moments to compute the parameters for the analytic PDF as a more direct way to recover the PDF than attempting to preserve the moments as in [5].

MCATK, the Monte Carlo Application Toolkit, was recently modified to tally final neutron and total fission numbers that result from individual source emission events over the length of the simulation as well as to source spontaneous fission neutrons or events [6]. The $S_N$neutral particle transport code PARTISN has the capability to compute the probability of initiation/survival (POI/POS) [7] and moments of the neutron number [5] and was recently modified to compute moments of the fission number as well. Here, we discuss the aforementioned 0-D transport analysis that allows us to approximate the PDF using information taken from full phase space transport solutions, the derivation and implementation of the stochastic transport equations for the moments of the cumulative fission number in PARTISN [8] and compare of the resulting PDFs with those generated with analog Monte Carlo using MCATK [9].

II. TRANSPORT MODELS

1. 0-D or 'Point' Model

The parameters utilized in a 0-D transport model or 'point-model' are the time-absorption eigenvalue

$$\alpha = \frac{\bar{\nu}\dot{F}_\alpha - \dot{L}_\alpha}{N_\alpha}, \tag{1a}$$

the related quantity k_α (not to be confused with k_{eff})

$$k_\alpha = \frac{\bar{\nu}\dot{F}_\alpha}{\dot{L}_\alpha} \tag{1b}$$

and the neutron lifetime

$$\tau_\alpha = \frac{N_\alpha}{\dot{L}_\alpha} = \frac{k_\alpha - 1}{\alpha} \tag{1c}$$

where $\bar{\nu}$ is the mean number of neutrons emitted in fission, $\dot{F}_\alpha$ and $\dot{L}_\alpha$ are the fission and loss (i.e., leakage and absorption) rates, respectively, and N_α is the total number of neutrons in the system. The lifetime as defined in (1c) is the mean time between loss events, α is indicative of the rate at which the neutron population grows and k_α is the ratio of neutrons in successive generations. Note that all of these parameters have been defined in terms of the α-eigenmode, as denoted by the subscript α.

The relation $\frac{\partial N}{\partial t} = \alpha N + \dot{S}$, where $\dot{S}$ is the source rate and N is the neutron number density, forms the basis for the point model, but its range of validity is limited. The α-eigenvalue and corresponding eigenmode are *time-asymptotic solutions to a source-less problem*; they describe how the neutrons in the system would behave if they were allowed to equilibrate in the absence of a neutron source. If the neutron population has not equilibrated to the α-eigenmode or if the source contributes appreciably to $\frac{\partial N}{\partial t}$ in relation to αN and is not distributed in the same way as the α-eigenmode, then the equation is not exact and may actually give significantly inaccurate estimates of the time behavior of the system.

Despite its limitations, however, the point-model allows for analytic solutions where they would not otherwise exist. For instance, reducing the stochastic transport equations to 0-D by integrating over space, angle and energy, and assuming, among other things, that the system is static in time yields an analytic expression for the probability density function (PDF) of the neutron number, n, which is asymptotically correct for large neutron numbers and the quadratic approximation [3]:

$$P_n(n) = \left(\frac{n}{\overline{n}}\right)^{\eta-1} \frac{\eta^\eta}{\overline{n}\Gamma(\eta)} e^{-\eta\frac{n}{\overline{n}}} \tag{2a}$$

$$\eta = \frac{2\dot{S}}{\chi_2'} = \frac{2\dot{S}\tau\bar{\nu}}{k_\alpha \chi_2} = \frac{\dot{S}\cdot POI_1}{\alpha} \tag{2b}$$

where $\overline{n}$ is the mean of n, $\bar{\nu}$ is the mean number of neutrons emitted in fission, $\chi_2 = \overline{\nu(\nu-1)}$ is twice the mean number of doublets emitted in fission and POI_1 is the static single neutron probability of initiation, given in this model as $POI_1 = \frac{2\alpha\tau\bar{\nu}}{k_\alpha\chi_2}$. This PDF is a gamma distribution with shape and rate parameters η and is therefore referred to in this document as the 'gamma' PDF (not to be confused with the gamma function). The higher-order moments of this distribution also have analytic representations:

$$\sigma_n = \frac{\overline{n}}{\sqrt{\eta}} \quad , \quad S_n = \frac{2}{\sqrt{\eta}} \quad , \quad \kappa_n = \frac{6}{\eta}. \tag{3}$$

where σ_n is the standard deviation, S_n is the skewness and κ_n is the excess kurtosis. Note that if the moments of the distribution are known and it is assumed that the gamma PDF has the correct shape, then the moments can be used to calculate η. Furthermore, the probability of exceeding a certain number of neutrons in the system is simply unity minus the CDF of the distribution:

$$P(n' > n) = \frac{1}{\Gamma(\eta)}\Gamma\left(\eta, \eta\frac{n'}{\overline{n}}\right) \tag{4}$$

where $\Gamma\left(\eta, \eta\frac{n}{\overline{n}}\right)$ is the upper incomplete gamma function.

It was also shown in [4] that for the point-model *at 'late' times* where $\alpha t \gg 1$, the neutron and fission numbers are perfectly correlated (i.e., there is a linear relationship between the total fission (f) and instantaneous neutron numbers) such that $f = an+b$, where $a = \sigma_f/\sigma_n$ and $b = \overline{f} - a\overline{n}$ are dependent on the first and second moments of each distribution:

$$\begin{aligned} P_f(f) &\approx \frac{\sigma_n}{\sigma_f}\left(\frac{\sigma_n}{\sigma_f}\frac{(f-\overline{f})}{\overline{n}} + 1\right)^{\eta-1} \frac{\eta^\eta}{\overline{n}\Gamma(\eta)} e^{-\eta\frac{\sigma_n}{\sigma_f}\left(\frac{(f-\overline{f})}{\overline{n}}+1\right)} \\ &= \frac{1}{a}\left(\frac{f-b}{a\overline{n}}\right)^{\eta-1} \frac{\eta^\eta}{\overline{n}\Gamma(\eta)} e^{-\eta\frac{(f-b)}{a\overline{n}}} \end{aligned} \tag{5}$$

where $\overline{f}$ is the mean of f and σ_n and σ_f are the standard deviations of n and f, respectively. This distribution preserves $\overline{f}$ and V_f exactly, but the skewness and excess kurtosis are the same as those for n, i.e., $S_f = S_n = \frac{2}{\sqrt{\eta}}$ and $\kappa_f = \kappa_n = \frac{6}{\eta}$. The probability of exceeding a certain number of fissions in the system is, again, a function of the upper incomplete gamma function:

$$P(f' > f) = \frac{1}{\Gamma(\eta)}\Gamma\left(\eta, \eta\frac{f'-b}{a\overline{n}}\right). \tag{6}$$

2. Full Phase-Space Fission Moment Equations

The equations for the moments of the fission number are derived using the same procedure as that for the neutron number [1]. We are interested in $P_f(V, t_f|\boldsymbol{r}, \boldsymbol{v}, t)$, the probability that a neutron introduced at $(\boldsymbol{r}, \boldsymbol{v}, t)$ (neutron location, velocity and time) will lead to f fissions in the volume V in the time interval $[t, t_f]$ where the probability of event x occurring per unit time on some small time interval Δt is related to Σ_x, the macroscopic cross section, by $v\Sigma_x(\boldsymbol{r}, \boldsymbol{v})\Delta t$. In the following equations, Σ_t, Σ_c, Σ_s and Σ_f are the total, capture, scattering and fission macroscopic cross sections and p_ν is the probability that ν neutrons are emitted in a fission event. All possible events that may occur in $[t, t+\Delta t]$ and lead to the desired outcome are then considered.

1. *No interaction:* Neutron was introduced at $(\boldsymbol{r}+\boldsymbol{v}\Delta t, \boldsymbol{v}, t + dt) \rightarrow$ Leads to f fissions on $[t+\Delta t, t_f]$

$$(1 - v\Sigma_t(\boldsymbol{r}+\boldsymbol{v})\Delta t)\, P_f(V, t_f|\boldsymbol{r}+\boldsymbol{v}\Delta t, \boldsymbol{v}, t+\Delta t) \tag{7a}$$

2. *Capture:* No fissions occur

$$v\Sigma_c(\boldsymbol{r}, \boldsymbol{v})\Delta t \delta_{f,0} \tag{7b}$$

3. *Scatter into $\boldsymbol{v}'$:* Scattered neutron emerges at $(\boldsymbol{r}+\boldsymbol{v}\Delta t, \boldsymbol{v}', t+\Delta t)$ and leads to f fissions on $[t+\Delta t, t_f]$

$$\Delta t \int d\boldsymbol{v}' v\Sigma_s(\boldsymbol{r}, \boldsymbol{v} \rightarrow \boldsymbol{v}') \cdot P_f(V, t_f|\boldsymbol{r}+\boldsymbol{v}\Delta t, \boldsymbol{v}', t+\Delta t) \tag{7c}$$

4. *Fission producing zero neutrons:* No further fissions occur

$$p_0 \cdot v\Sigma_f(\boldsymbol{r}, \boldsymbol{v})\Delta t \cdot \delta_{f,1} \tag{7d}$$

5. *Fission producing one neutron:* Neutron emerges at $(\boldsymbol{r} + \boldsymbol{v}\Delta t, \boldsymbol{v}'_1, t + \Delta t)$ and leads to $(f-1)$ fissions on $[t + \Delta t, t_f]$

$$p_1 \cdot v\Sigma_f(\boldsymbol{r},\boldsymbol{v})\Delta t \cdot \int d\boldsymbol{v}'_1 \chi(\boldsymbol{v} \to \boldsymbol{v}'_1) \cdot P_{f-1}(V, t_f|\boldsymbol{r} + \boldsymbol{v}\Delta t, \boldsymbol{v}'_1, t + \Delta t) \quad (7e)$$

where $\chi(\boldsymbol{v} \to \boldsymbol{v}'_1)$ is the probability that a fission induced by a neutron with velocity $\boldsymbol{v}$ releases a neutron with velocity $\boldsymbol{v}'_1$

6. *Fission producing two neutrons:* Neutrons emerge at $(\boldsymbol{r} + \boldsymbol{v}\Delta t, \boldsymbol{v}'_1, t + \Delta t)$ and $(\boldsymbol{r} + \boldsymbol{v}\Delta t, \boldsymbol{v}'_2, t + \Delta t)$ and, together, lead to $(f-1)$ fissions on $[t + \Delta t, t_f]$

$$p_2 \cdot v\Sigma_f(\boldsymbol{r},\boldsymbol{v})\Delta t \cdot \sum_{f_1}\sum_{\substack{f_2 \\ f_1+f_2=(f-1)}} \int d\boldsymbol{v}'_1 \int d\boldsymbol{v}'_2 \chi(\boldsymbol{v} \to \boldsymbol{v}'_1)\chi(\boldsymbol{v} \to \boldsymbol{v}'_2) \cdot P_{f_1}(V, t_f|\boldsymbol{r} + \boldsymbol{v}\Delta t, \boldsymbol{v}'_1, t + \Delta t) \cdot P_{f_2}(V, t_f|\boldsymbol{r} + \boldsymbol{v}\Delta t, \boldsymbol{v}'_2, t + \Delta t) \quad (7f)$$

where it is assumed that there is no correlation between the velocities of the released neutrons

7. *Fission producing ν neutrons up to ν_{max}:* Neutrons emerge at $(\boldsymbol{r} + \boldsymbol{v}\Delta t, \boldsymbol{v}'_1, t + \Delta t)$, $(\boldsymbol{r} + \boldsymbol{v}\Delta t, \boldsymbol{v}'_2, t + \Delta t)$...$(\boldsymbol{r} + \boldsymbol{v}\Delta t, \boldsymbol{v}'_\nu, t + \Delta t)$ and, together, lead to $(f-1)$ fissions on $[t + \Delta t, t_f]$

$$p_\nu \cdot v\Sigma_f(\boldsymbol{r},\boldsymbol{v})\Delta t \cdot \sum_{f_1}\sum_{f_2}\cdots\sum_{\substack{f_\nu \\ f_1+f_2+\ldots+f_\nu=(f-1)}} \prod_{i=1}^{\nu} \int d\boldsymbol{v}'_i \chi(\boldsymbol{v} \to \boldsymbol{v}'_i) \cdot P_{f_i}(V, t_f|\boldsymbol{r}+\boldsymbol{v}\Delta t, \boldsymbol{v}'_i, t+\Delta t) \quad (7g)$$

Accumulating terms and taking the limit as $\Delta t \to 0$ yields and equation for $P_f(V, t_f|\boldsymbol{r},\boldsymbol{v},t)$:

$$-\frac{\partial P_f}{\partial t} - \boldsymbol{v} \cdot \nabla P_f + v\Sigma_t P_f = v\Sigma_c \delta_{f,0} + v\Sigma_s \int d\boldsymbol{v}' f(\boldsymbol{v} \to \boldsymbol{v}')P_f(V, t_f|\boldsymbol{r},\boldsymbol{v}',t) + v\Sigma_f p_0 \delta_{f,1} + v\Sigma_f \sum_{\nu=1}^{\nu_{max}} p_\nu \left(\sum_{f_1}\sum_{f_2}\cdots\sum_{\substack{f_\nu \\ f_1+f_2+\ldots+f_\nu=(f-1)}} \prod_{i=1}^{\nu} \int d\boldsymbol{v}'_i \chi(\boldsymbol{v} \to \boldsymbol{v}'_i) \cdot P_{f_i}(V, t_f|\boldsymbol{r} + \boldsymbol{v}\Delta t, \boldsymbol{v}'_i, t + \Delta t) \right). \quad (8a)$$

The final and boundary conditions reflect the observation that neutrons introduced at the final time or exiting the problem domain cannot lead to fission:

$$P_f(V, t_f|\boldsymbol{r},\boldsymbol{v},t_f) = \delta_{f,0} \quad (8b)$$

$$P_f(V, t_f|\boldsymbol{r}_B,\boldsymbol{v},t) = \delta_{f,0}, \quad \hat{\boldsymbol{\Omega}} \cdot \boldsymbol{n}_B > 0 \quad (8c)$$

An equation for the modified probability generating function, $\mathcal{G}(V, t_f|\boldsymbol{r},\boldsymbol{v},t;z) = 1 - \sum_{f=0}^{\infty} P_f(V, t_f|\boldsymbol{r},\boldsymbol{v},t)z^f$, can be generated by multiplying Eq. (8) by z^f and summing over all f:

$$-\frac{1}{v}\frac{\partial \mathcal{G}}{\partial t} - \hat{\boldsymbol{\Omega}} \cdot \nabla\mathcal{G} + \Sigma_t(\boldsymbol{r},\boldsymbol{v})\mathcal{G} = \int d\boldsymbol{v}'\Sigma_s(\boldsymbol{r},\boldsymbol{v} \to \boldsymbol{v}')\mathcal{G}(V, t_f|\boldsymbol{r},\boldsymbol{v}',t) + z\Sigma_f(\boldsymbol{r},\boldsymbol{v}) \sum_{\nu=0}^{\nu_{max}} p_\nu \left[\int d\boldsymbol{v}'\chi(\boldsymbol{v} \to \boldsymbol{v}')\mathcal{G}(V, t_f|\boldsymbol{r},\boldsymbol{v}',t) \right]^\nu \quad (9a)$$

$$\mathcal{G}(V, t_f|\boldsymbol{r},\boldsymbol{v},t_f;z) = 0 \quad (9b)$$

$$\mathcal{G}(V, t_f|\boldsymbol{r}_B,\boldsymbol{v},t;z) = 0, \quad \hat{\boldsymbol{\Omega}} \cdot \boldsymbol{n}_B > 0 \quad (9c)$$

Taking derivatives of this equation with respect to the generating function parameter z and setting $z = 1$ yields equations for the moments of the distribution. The equation for each moment is identical in form to the other moments of the fission number as well as the moments of the neutron number: They are standard linear adjoint transport equations with a source term, S_k, that depends on only the lower-order moments, therefore they are linear and coupled to the other moment equations unidirectionally and can therefore be solved sequentially.

$$\left(-\frac{1}{v}\frac{\partial}{\partial t} - \hat{\boldsymbol{\Omega}} \cdot \nabla + \Sigma_t(\boldsymbol{r},\boldsymbol{v},t)\right)\overline{f^k}(\boldsymbol{r},\boldsymbol{v},t) = \int d\boldsymbol{v}'\ \Sigma_s(\boldsymbol{r},\boldsymbol{v} \to \boldsymbol{v}',t)\overline{f^k}(\boldsymbol{r},\boldsymbol{v}',t) + \bar{\nu}\Sigma_f(\boldsymbol{r},\boldsymbol{v},t) \int d\boldsymbol{v}'\ \chi(\boldsymbol{v} \to \boldsymbol{v}')\overline{f^k}(\boldsymbol{r},\boldsymbol{v}',t) + S_k\left(\boldsymbol{r},\boldsymbol{v},t;\ \overline{f} \cdots \overline{f^{k-1}}\right) \quad (10a)$$

$$\overline{f^k}(\boldsymbol{r},\boldsymbol{v},t_f) = 0 \quad (10b)$$

$$\overline{f^k}(\boldsymbol{r}_B,\boldsymbol{v},t) = 0, \quad \hat{\boldsymbol{\Omega}} \cdot \boldsymbol{n}_B \geq 0 \quad (10c)$$

where $\overline{f^k}$ is the k^{th} moment of the fission number PDF for a single neutron emitted at $(\boldsymbol{r},\boldsymbol{v},t)$; t_f and $\boldsymbol{n}_B$ are the final time and unit normal to the system boundary. The sources, S_k, are given in Table I.

To get the moments of the fission distribution for a source, a second generating function equation is necessary:

$$G_S(z) = \exp\left(-\int d\boldsymbol{r} \int d\boldsymbol{v} \int_0^{t_f} dt \cdot S(\boldsymbol{r},\boldsymbol{v},t)\mathcal{G}(z;\boldsymbol{r},\boldsymbol{v},t)\right) \quad (11)$$

Once again, taking derivatives and setting $z = 1$ yields auxiliary equations for the mean, variance, skewness and excess kurtosis:

$$\overline{F} = E(F) = \int d\boldsymbol{r} \int d\boldsymbol{v} \int_0^{t_f} dt\, S(\boldsymbol{r},\boldsymbol{v},t)\overline{f^{(}}\boldsymbol{r},\boldsymbol{v},t) \quad (12a)$$

$$V_F = E\left((F - \overline{F})^2\right) = \int d\boldsymbol{r} \int d\boldsymbol{v} \int_0^{t_f} dt\, S(\boldsymbol{r},\boldsymbol{v},t)\overline{f^2}(\boldsymbol{r},\boldsymbol{v},t) \quad (12b)$$

k	$S_k(\boldsymbol{r}, \boldsymbol{v}, t)$
1	Λ_0
2	$\Lambda_0 + 2\left\langle\overline{f}\right\rangle\left(\Lambda_1 + \Lambda_2\left\langle\overline{f}\right\rangle\right)$
3	$\Lambda_0 + \left(3\Lambda_1 + 6\Lambda_2\left\langle\overline{f}\right\rangle\right)\left(\left\langle\overline{f}\right\rangle + \left\langle\overline{f^2}\right\rangle\right) + 6\Lambda_3\left\langle\overline{f}\right\rangle^3$
4	$\Lambda_0 + \Lambda_1\left(4\left\langle\overline{f^3}\right\rangle + 6\left\langle\overline{f^2}\right\rangle + 4\left\langle\overline{f}\right\rangle\right) + \Lambda_2\left(4\left\langle\overline{f}\right\rangle\left(2\left\langle\overline{f^3}\right\rangle + 6\left\langle\overline{f^2}\right\rangle + 3\left\langle\overline{f}\right\rangle\right) + 6\left\langle\overline{f^2}\right\rangle^2\right)$ $+12\,\Lambda_3\left\langle\overline{f}\right\rangle^2\left(3\left\langle\overline{f^2}\right\rangle + 2\left\langle\overline{f}\right\rangle\right) + 24\,\Lambda_4\left\langle\overline{f}\right\rangle^4$

TABLE I. **The inhomogeneous source, S_k, for** (10a) **for $k = 1, 2, 3\,\&\,4$, where** $\Lambda_i(\boldsymbol{r}, \boldsymbol{v}, t) = \frac{\Sigma_f(\boldsymbol{r},\boldsymbol{v},t)}{i!}\sum_{j=i}^{I}\frac{j!}{(j-i)!}p_j(\boldsymbol{r}, \boldsymbol{v}, t)$**,** p_j **is the probability that** j **neutrons are emitted in a fission event and** $\left\langle f^k\right\rangle = \int dv'\,\chi(v \to v')\overline{f^k}(v')$**.**

$$s_F = \frac{E\left((F-\overline{F})^3\right)}{\left[E\left((F-\overline{F})^2\right)\right]^{3/2}} = \frac{\int d\boldsymbol{r}\int d\boldsymbol{v}\int_0^{t_f} dt\, S(\boldsymbol{r},\boldsymbol{v},t)\overline{f^3}(\boldsymbol{r},\boldsymbol{v},t)}{V_F^{3/2}} \tag{12c}$$

$$\kappa_F = \frac{E\left((F-\overline{F})^4\right)}{\left[E\left((F-\overline{F})^2\right)\right]^2} - 3 = \frac{\int d\boldsymbol{r}\int d\boldsymbol{v}\int_0^{t_f} dt\, S(\boldsymbol{r},\boldsymbol{v},t)\overline{f^4}(\boldsymbol{r},\boldsymbol{v},t)}{V_F^2}. \tag{12d}$$

Here, only the first four moments are considered, but it is possible to obtain as many moments as may be useful. As can be seen, these equations are *auxiliary* equations—the source is not represented explicitly in the transport-like equations, but is instead incorporated into the solution after the fact. The relationship between the single neutron and source moments are the same as those for the neutron number given in [5].

III. RESULTS AND ANALYSIS

Previously, the gamma PDF for n and the mapping of that PDF to the fission number f were found to agree well with PDFs generated using 0-D Monte Carlo [4]. Here, the gamma PDF for n and corresponding mapping to the PDF for f are compared against full phase-space transport codes. To make code comparisons straightforward, the first test case is a static bare Plutonium sphere with a fast neutron spectra ("Jezebel"). The results of many MCATK analog Monte Carlo 'experiments' are tallied to generate PDFs and cumulative density functions (CDFs), which can then be compared against (2a) and (5). MCATK and PARTISN are both used to compute the moments of the neutron and fission numbers. The second is a bare Uranium sphere with time-varying isotopic abundances of U-235 and U-238 and demonstrates the applicability of our method to dynamic systems.

1. Plutonium Sphere

This test problem is a 6.5 cm sphere of enriched Plutonium with the same isotopic concentrations as Jezebel (95.5$^w/_o$ Pu-239, 4.5$^w/_o$ Pu-240). The total spontaneous fission rate is $\dot{S}$=0.847254/μs. In MCATK, only the dominant Pu-240 spontaneous fission source is used, so the source rate is slightly ($\approx$ 0.03%) lower: $\dot{S}$=0.846996/μs. In Table II, results are shown for PARTISN for various numbers of energy groups, G. Results are given for α, single neutron POI (POI_1) and k. Also shown is the parameter η computed using the POI and α as computed in the 0-D analysis and the first two moments of the distribution taken from the full phase space model. As can be seen, they differ with the latter being always smaller. For MCATK, only the eigenvalues are computed. The simulation was run for 0.5 μs, at the end of which the instantaneous average neutron number, $\overline{n}$, and the average number of fission events , $\overline{f}$, are reported. For all MCATK simulations, the source is time-biased (and appropriately weighted) such that equal numbers of neutrons are emitted for each of 4 time intervals: $[0.0, 0.03, 0.1, 0.2, 0.5]$ μs.

As can be seen in Table II, PARTISN α and $\overline{n}$ appear to be approaching the MCATK results from below up to G = 30. At G = 133, however, these quantities jump up above the MCATK value and then approach them from above as the number of energy groups in increased. For this problem, $\bar{\nu}$ = 3.002549, and it can be seen that $\bar{\nu}\overline{f}$ for MCATK is approximately equal to $\overline{f}_{prod}$ as reported by PARTISN.

Table III shows the first four central moments of n as well as the probability that there will be more than n neutrons in the system at the final time—i.e., $P(n' > n) = \int_n^\infty dn'\, P_n(n')$. The 'converged' 133 group PARTISN calculation overestimates the mean and probability of $n' > n$ for large n, but the rest of the results are close to the MCATK results. The 'unconverged' 12 group calculation tends to underestimate all quantities, but the 21 group calculation is an excellent (and indeed the best) match to MCATK. Once again, the gamma PDFs generated using the MCATK values of η do not exactly reproduce the skewness and kurtosis, indicating that the PDF is not exactly a gamma distribution, but they do reproduce $P(n' > n)$ reasonably well.

Table IV shows the mapping parameters and moments and $P(f' > f)$ for MCATK. As can be seen, and as expected, the first two moments match exactly between the PDF and the tally and the PDF matches the tally quite well on $P(f' > f)$ *for large* f. There are larger differences in the skewness and kurtosis as well as the $P(f' > f)$ for small f.

Figures 1 and 2 show the PDFs and complements of the CDFs of n and f for the MCATK tally and the gamma distribution generated using the MCATK and PARTISN moments. The gamma PDFs agree and, additionally, match the MCATK results well for n and large f, although a more rigorous comparison is available in Tables III and IV. The mapping breaks down for small f, however. This is expected because neutron chains that die prior to the final time are not represented in

code	G	α (μs^{-1})	POI_1	$\eta = \frac{\dot{S} \cdot POI_1}{\alpha}$	$\eta = \frac{\overline{n}^2}{V_n}$	k	$\overline{n}$	$\overline{f}$
PARTISN	618	7.79317	1.3541E-2	1.4721E-3	1.4195E-3	1.02207	6.05114	63.0430
	250	7.79475	1.3549E-2	1.4727E-3	1.4195E-3	1.02208	6.05410	63.0516
	133	7.79563	1.3565E-2	1.4743E-3	1.3967E-3	1.02211	6.05525	63.0084
	30	7.71853	1.3687E-2	1.5024E-3	1.3955E-3	1.02230	5.86632	60.6259
	21	7.71843	1.3687E-2	1.5024E-3	1.3951E-3	1.02230	5.86611	60.6247
	12	7.40690	1.3381E-2	1.5306E-3	1.4498E-3	1.02177	5.19236	54.5328
MCATK	–	7.72534			1.3641E-3	1.02182	5.86592	61.4381

TABLE II. Pu Sphere: Static parameters and means at $t_f = 0.5\,\mu s$. PARTISN parameters: 0.25 mm mesh ($I = 260$), S-256 quadrature & P-4 scattering. 20.48 million time-biased MCATK source neutrons (singlet emitting). ENDF-VII.1 cross section data.

	MCATK		PARTISN		
	tally	PDF	$G = 133$	$G = 21$	$G = 12$
η	–	1.36411E-3	1.39669E-3	1.41948E-3	1.44981E-3
$\overline{n}$	5.86592E0	5.86592E0	6.05525E0	5.86611E0	5.19236E0
σ_n	1.58931E2	1.58931E2	1.62025E2	1.55699E2	1.36367E2
S_n	5.59415E1	5.41509E1	5.48005E1	5.44097E1	5.37917E1
κ_n	4.78018E3	4.39848E3	4.56881E3	4.50578E3	4.40186E3
$P(n' > 1E2)$	4.47437E-3	4.36682E-3	4.48202E-3	4.48887E-3	4.38330E-3
$P(n' > 1E3)$	1.49215E-3	1.50210E-3	1.54701E-3	1.51861E-3	1.39124E-3
$P(n' > 5E3)$	2.24050E-4	2.29647E-4	2.38725E-4	2.21729E-4	1.69809E-4
$P(n' > 1E4)$	4.29246E-5	4.29475E-5	4.51026E-5	3.94188E-5	2.47497E-5

TABLE III. Pu Sphere: Moments of n and probability that there are more than n neutrons ($P(n' > n)$) at $t_f = 0.5\,\mu s$. Results are given for MCATK using the tally ("tally") and for MCATK and PARTISN using (2a) where $\eta = \frac{\overline{n}^2}{V_n}$. 20.48 million MCATK source neutrons

the neutron number PDF on which the fission number PDF is based. These chains have produced fissions, however, and therefore contribute to the fission number PDF, predominantly in the low fission number range as can be seen. This discrepancy is therefore unavoidable without incorporating information about the neutron number at earlier times. If we are interested in the probability of getting large numbers of fission and therefore dose, then this limitation is acceptable.

2. Uranium Sphere with Varying Isotopic Abundance

The second test problem is a modification of a test problem from [7] and is a mockup of a criticality accident scenario. The system is a 17.25 cm sphere with a time-varying mixture of U^{235} and U^{238} where $\rho_{235} = 14 - 6C_{mod}$ g/cm^3 and $\rho_{238} = 1 + 6C_{mod}$ g/cm^3, where C_{mod} varies linearly between the time points shown in Table V. The system was modeling using the MENDF71x data library with NDI's 133 group set, 120 spatial cells, S_{20} and P_3 and there is a uniformly distributed volume source in group 7 (14-14.25 MeV) emitting a total of 0.1 n/μs.

Figure 3 shows the gamma PDF η parameter computed using the moments and the various definitions from Eq. (3). There are only slight differences between the three definitions, which assume a gamma distribution, so this result indicates that the PDF is very nearly a gamma distribution. It also becomes fixed at a constant value before the system becomes supercritical indicating that, while the neutron population may fluctuate, the shape of the distribution is fixed. η was also computed using the POI and α from static snapshots. As can be seen, it varies with time, which incorrectly indicates that the shape of the distribution is changing over the course of the excursion.

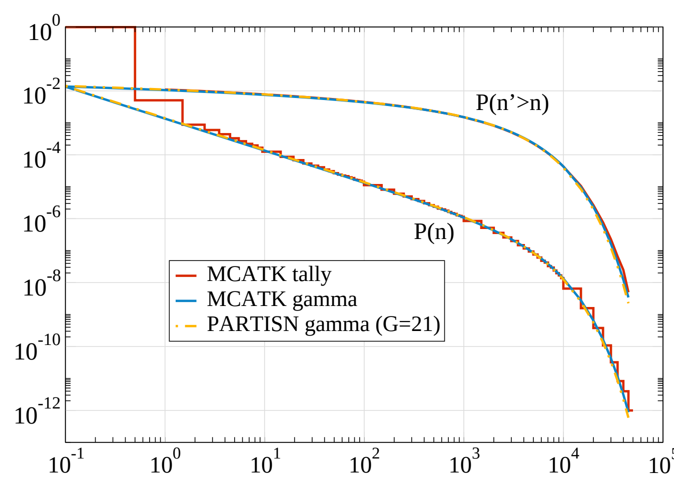


Fig. 1. Pu Sphere: Comparison of neutron number distributions where $\eta = \frac{\overline{n}^2}{V_n}$ are computed using the moments.

	MCATK		PARTISN		
	tally	PDF	G = 133	G = 21	G = 12
a	–	1.01582E1	1.01082E1	1.03410E1	1.01666E1
b	–	1.85088E0	1.80076E0	1.76354E0	1.74410E0
$\overline{f}$	6.14381E1	6.14381E1	6.30084E1	6.06247E1	5.45328E1
σ_f	1.61335E3	1.61335E3	1.63778E3	1.56230E3	1.38639E3
S_f	5.60809E1	5.41509E1	5.50093E1	5.46317E1	5.40205E1
κ_f	4.81119E3	4.39848E3	4.60910E3	4.54827E3	4.44557E3
$P(f' >$1E2)	1.15902E-2	7.50749E-3	7.68992E-3	7.77905E-3	7.71456E-3
$P(f' >$1E3)	4.66869E-3	4.39011E-3	4.49909E-3	4.53758E-3	4.40895E-3
$P(f' >$1E4)	1.50379E-3	1.51928E-3	1.55914E-3	1.55628E-3	1.40957E-3
$P(f' >$5E4)	2.30942E-4	2.38600E-4	2.43519E-4	2.36244E-4	1.75829E-4
$P(f' >$1E5)	4.53086E-5	4.59624E-5	4.66239E-5	4.38380E-5	2.62571E-5

TABLE IV. Pu Sphere: Moments of f for $t \in (0, 0.5)$. Results are given for MCATK for the mapped gamma (i.e., the mapped distribution given in (5) and $\eta = \frac{\overline{n}^2}{V_n}$: "PDF") and using the tally ("tally").

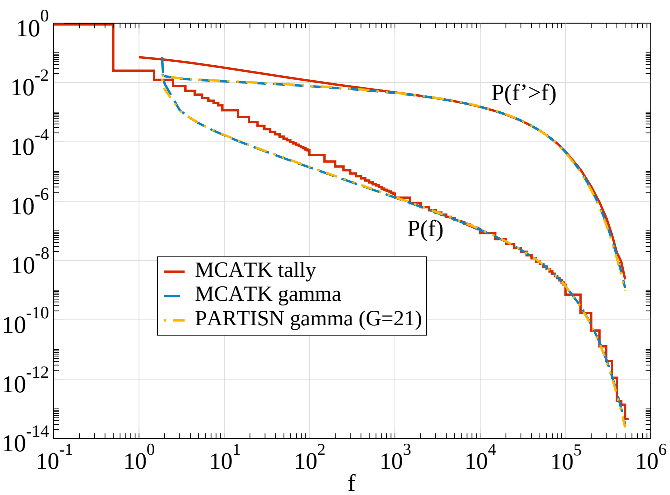


Fig. 2. Pu Sphere: Comparison of fission number distributions where $\eta = \frac{\overline{n}^2}{V_n}$, $a = \sigma_f/\sigma_n$ and $b = \overline{f} - a\overline{n}$ are computed using the moments.

Figure 4 shows the means of n and f as computed using the forward and moment equations. Since PARTISN outputs fission production rate, not fission rate, the forward fission result is divided by 2.5, which is roughly equivalent to $\overline{\nu}$ for Uranium. The two calculation methods agree well, as would be expected.

Table VI shows the moments and PDF parameters for two time points: Second critical (3.5 μs) and once the number of fissions has stopped increasing (5.0 μs). Note that $S_n \approx S_f$ and $\kappa_n \approx \kappa_f$, which is also true of the analytic representations of P_n and P_f. These parameters are then used to plot the PDFs and the complements of the CDFs (i.e., the probability of exceeding n neutrons or f fissions) in Figure 5. MCATK results were not available at submission time, but will be presented at the conference. Once again, P_f is reasonable in the tail, but is clearly incorrect for small fission numbers where the mapping breaks down. As previously stated, we are generally interested in the probability of getting large numbers

time(μs)	C_{mod}
0.0	1.5
1.0	1.25
2.0	0.625
2.5	0.625
3.5	1.25
>4.5	1.5

TABLE V. C_{mod} Parameter for Uranium Sphere

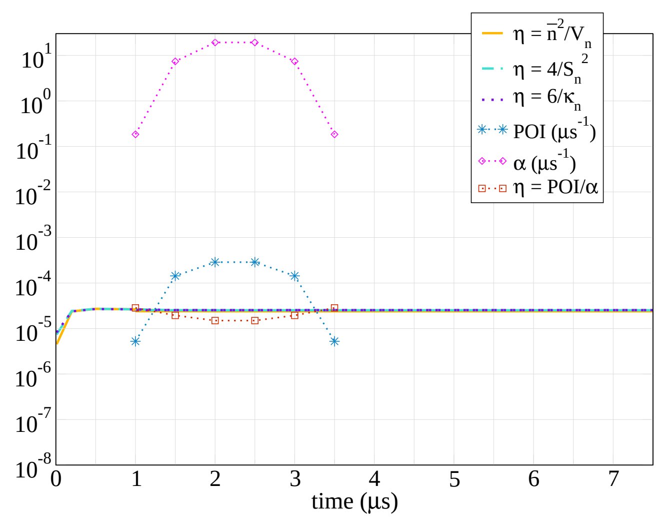


Fig. 3. U Sphere: Gamma PDF parameter η computed using the various moments of n (see Eq. (3)) and the point model.

of neutrons and fissions, so this is an acceptable limitation.

IV. CONCLUSIONS

When moments of the neutron number distribution are computed using PARTISN and MCATK and used to estimate the shape parameter, η, of the analytic gamma PDF, the PDF compares well with the MCATK tally. When the mapped analytic gamma PDF for fission number is generated in the

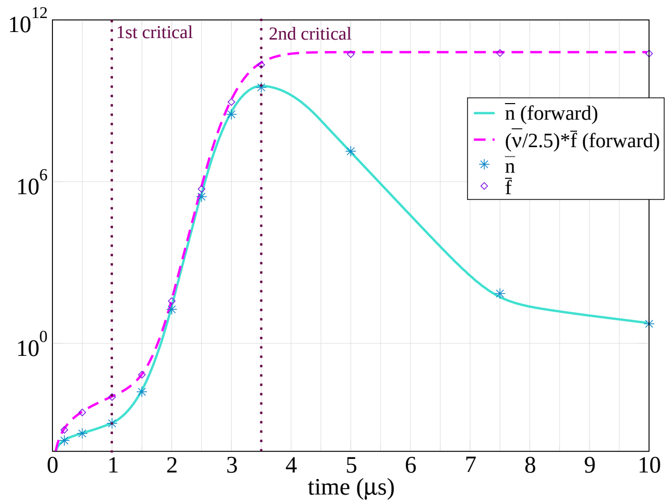
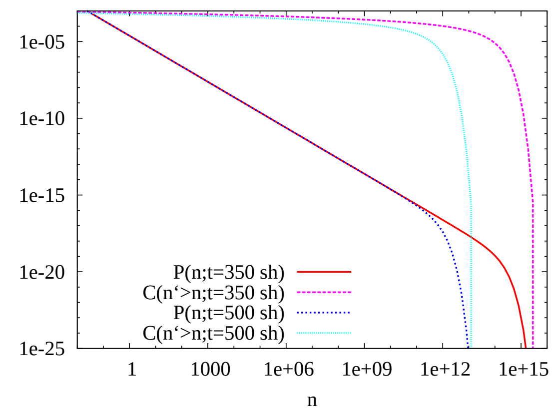


Fig. 4. U Sphere: Comparison of $\overline{n}$ and $\overline{f}$ for the forward and moment equations.

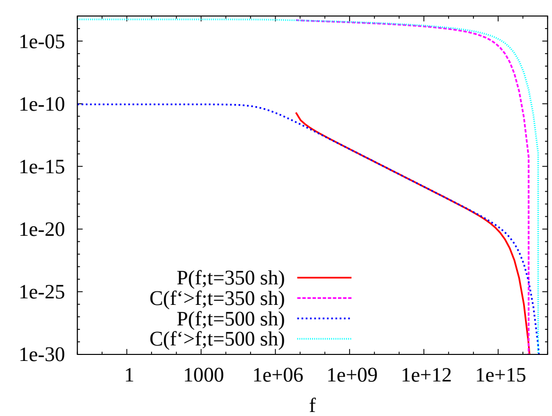
	simulation time (μs)	
	3.5	5.0
η	2.39632E-5	2.39735E-5
$\overline{n}$	3.13589E9	1.33739E7
σ_n	6.40603E11	2.73145E9
S_n	3.98380E2	3.98345E2
κ_n	2.36486E5	2.36547E5
a	6.81167	4.00332E3
b	5.52567E6	-2.67668E5
$\overline{f}$	2.13662E10	5.35400E10
σ_f	4.36358E12	1.09349E13
S_f	3.98428E2	3.98296E2
κ_f	2.36585E5	2.36477E5

TABLE VI. U Sphere: Moments and PDF parameters.

same way, it is also found to compare well with the MCATK tally *in the tail of the distribution* where the mapping is valid. Overall, though, for this class of problems (slightly supercritical bare metal spheres), the generated PDFs were good representations of the actual distributions.



(a) PDF and complement of the CDF of n



(b) PDF and complement of the CDF of f

Fig. 5. U Sphere: PDFs and complements of the CDFs at 3.5 and 5.0 μs.

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