LA-12570

Analytic Score Distributions and Moments for a Spatially Continuous Tridirectional Monte Carlo Transport Problem

Los Alamos
NATIONAL LABORATORY

Los Alamos National Laboratory is operated by the University of California for the United States Department of Energy under contract W-7405-ENG-36.

Edited by Patricia W. Mendius, Group IS-1
Prepared by M. Ann Nagy, Group X-6

LA-12570

UC-905 and UC-705
Issued: July 1993

Analytic Score Distributions and Moments for a Spatially Continuous Tridirectional Monte Carlo Transport Problem

Thomas E. Booth

MASTER

Los Alamos
NATIONAL LABORATORY
Los Alamos, New Mexico 87545

ANALYTIC SCORE DISTRIBUTIONS AND MOMENTS FOR A SPATIALLY CONTINUOUS TRIDIRECTIONAL MONTE CARLO TRANSPORT PROBLEM

by

Thomas E. Booth

ABSTRACT (U)

The interpretation of the statistical error estimates produced by Monte Carlo transport codes is still somewhat of an art. Empirically, there are variance reduction techniques whose error estimates are almost always reliable and there are variance reduction techniques whose error estimates are *often* unreliable. Unreliable error estimates usually result from inadequate large score sampling from the score distribution's tail.

Statisticians believe that more accurate confidence interval statements are possible if the general nature of the score distribution can be characterized. This paper provides the analytic score distribution for the exponential transform applied to a simple spatially continuous Monte Carlo transport problem.

I. INTRODUCTION

The Radiation Transport Group and the Statistics Group at the Los Alamos National Laboratory are involved in a collaborative research project whose motivation is to obtain better confidence intervals for Monte Carlo transport calculations.

The statisticians have repeatedly emphasized that the more information they had about the general nature of the score distributions, the better they could make the confidence intervals. The statisticians sought both empirical data from our Monte Carlo computer code (MCNP[1]) and exact theoretical results to guide them in their attempt to provide better confidence intervals. Empirical results[2,3] are described elsewhere by the author's collaborators, R. A. Forster of the Radiation Transport Group and S. P. Pederson of the Statistics Group. This note describes some theoretical results desired by the statisticians.

Modern Monte Carlo particle transport codes (e.g., MCNP) offer the user a wide variety of variance reduction techniques. These techniques change the score distribution from the physical distribution. For example, if one counts the number of physical neutrons penetrating a nonmultiplying shield, then for each incident neutron either one neutron penetrates the shield with probability p, or zero neutrons penetrate with probability $1-p$. The natural variance of this binomial process is $p-p^2$. One may not know the value of p, but one knows *the form* of the score distribution. However, when variance reduction techniques are used, *the form* of the score distribution usually is not known. This problem is significant when confidence intervals are desired.

The error estimates in a Monte Carlo calculation are reliable only when sufficient numbers of large scores have been sampled. In an analog calculation of the penetration problem one *knows* how many large (i.e., score=1) scores have been sampled. A statistical error estimate is relatively easy in this case because the score distribution is known except for the exact value of the binomial parameter p. By contrast, very little theory exists concerning the form, or general behavior, of the score distribution when variance reduction techniques are used. Standard statistical estimates in Monte Carlo codes are based almost always only on the sampled scores with little consideration given to the impact of the scores that were not sampled.

This work is not intended to supply Monte Carlo practitioners with practical suggestions for picking variance reduction parameters. The interested reader can consult references 4 and 5 for this purpose. The importance of this work lies in the fact that statisticians now have an exact score distribution arising from a common Monte Carlo technique to test alternative ways of obtaining confidence intervals.

The exponential transform is an old and widely used variance reduction technique. References 4 and 5 summarize much of the knowledge about the exponential transform. Recently, an exponential transform technique was applied to a simple, discrete, two-state transport problem[6–8] and the exact analytic score distribution was obtained. Because the same mechanisms create weight fluctuations in the discrete problem and a continuous problem, it was conjectured that the general nature of the score distribution would be similar for a continuous transport problem. This paper derives the exact analytic score distribution for a spatially continuous transport problem with the exponential transform and shows that the *form* of the score distribution is indeed *very* similiar in the discrete and continuous transform cases.

This paper proceeds by deriving the score moment equations for a simple three direction spatially continuous slab penetration problem. The derivation of the score moment equations is not new and reference 5 provides a far more general derivation than is provided here. In addition, reference 5 provides a good source of references for the historical development and use of the moment equations. The equations are rederived here for three reasons. First, the derivation is not difficult and there is no more work involved than in simplifying the general equations to the simple case herein. Second, the style of the derivation provides an introduction to the derivation of the score distribution equations. Third, the present paper is easier to read because it is self-contained and does not have to explain the terms required to treat more complicated problems before simplifying to the case herein.

II. DESCRIPTION OF TEST PROBLEM

The test problem consists of a slab of thickness T, with a normally incident source at the $x = 0$ surface of the slab, and a tally that simply counts the weight penetrating the $x = T$ outside surface of the slab. The particles always move parallel, antiparallel, or perpendicular to the x-axis; thus, there are only three possible particle directions.

III. DERIVATION OF THE SCORE MOMENT EQUATIONS

The physical state of a particle in this simple test problem is determined by its x position and its direction either parallel, antiparallel, or perpendicular to the x-axis. In addition, the particle will carry a statistical weight w. A few definitions are required before deriving the score probability equations.

Definition 1. $\eta(x,s,w)ds$ = the probability that a particle of weight w moving perpendicular to the $\hat{x}$ direction scores s in an interval ds about s.

Definition 2. $\phi(x,s,w)ds$ = the probability that a particle of weight w moving in the $+\hat{x}$ direction scores s in an interval ds about s.

Definition 3. $\psi(x,s,w)ds$ = the probability that a particle of weight w moving in the $-\hat{x}$ direction scores s in an interval ds about s.

Definition 4. σ = total macroscopic cross section

Definition 5. σ_s = macroscopic scattering cross section.

Definition 6. p = exponential transform parameter.

The exponential transform uses a fictitious total cross section $\sigma_{transform} = (1 - p\mu)\sigma$, where μ is the direction cosine with respect to the x-axis. This paper allows a slightly more general treatment in that the fictitious total cross section can be arbitrarily specified in three directions ($\mu = \{-1, 0, 1\}$). The cross sections for particles moving in the positive, perpendicular, and negative directions are

$$\sigma_+ = \text{fictitious total cross section in the} + \hat{x} \text{ direction} \tag{1}$$

$$\sigma_0 = \text{fictitious total cross section in the direction perpendicular to } \hat{x} \tag{1.1}$$

$$\sigma_- = \text{fictitious total cross section in the} - \hat{x} \text{ direction} \tag{2}$$

Let s be the distance the particle moves between events (either collisions or surface crossings). The exponential transform events are weighted by[1]:

$$w_{event} = \frac{\text{true probability of event}}{\text{sampled probability of event}} \tag{3}$$

The weight multiplication upon collision for a particle moving in the $+\hat{x}$ direction is:

$$w_+ = \frac{\sigma e^{-\sigma s}}{\sigma_+ e^{-\sigma_+ s}} \tag{4}$$

The weight multiplication upon collision for a particle moving in the $-\hat{x}$ direction is:

$$w_- = \frac{\sigma e^{-\sigma s}}{\sigma_- e^{-\sigma_- s}} \tag{5}$$

The weight multiplication upon collision for a particle perpendicular to the $\hat{x}$ direction is:

$$w_0 = \frac{\sigma e^{-\sigma s}}{\sigma_0 e^{-\sigma_0 s}} \tag{5.1}$$

The weight multiplication upon crossing $x = T$ is:

$$w_T = \frac{e^{-\sigma s}}{e^{-\sigma_+ s}} \tag{6}$$

The scattering probabilities for forward, 90 degree, and backward scatterings are:

$$f = \text{probability of no direction change upon scatter} \tag{6.1}$$

$$q = \text{probability of scattering perpendicularly} \tag{6.2}$$

$$b = \text{probability of direction reversal upon scatter} \tag{6.3}$$

Using Eqs. 1-6.3. the score probability equations with the exponential transform can be derived.

Later in this paper, the score probability equations with the exponential transform *and* survival biasing (implicit capture) will be desired. The derivations are very similiar and need not be done twice. For the current case of analog capture set,

$$v \doteq 1 \tag{6.4}$$

$$g \doteq \frac{\sigma_s}{\sigma} \tag{6.5}$$

The score probability equations are written and then explained below.

$$\phi(x, s, w)ds = \left[\int_x^T \sigma_+ e^{-\sigma_+(y-x)}\left\{g\left[f\phi(y, s, w_+vw) + q\eta(y, s, w_+vw)\right.\right.\right.$$
$$\left.\left.\left. + b\psi(y, s, w_+vw)\right] + \frac{\sigma_a}{\sigma}\delta(s)\right\}dy + e^{-\sigma_+(T-x)}\delta(s - ww_T)\right]ds \tag{7}$$

$$\eta(x,s,w)ds = \int_0^\infty \sigma_0 e^{-\sigma_0 z}\Big\{g[\frac{q}{2}\phi(x,s,vw) + (f+b)\eta(x,s,vw) + \frac{q}{2}\psi(x,s,vw)] + \frac{\sigma_a}{\sigma}\delta(s)\Big\}dz ds \tag{8}$$

$$\psi(x,s,w)ds = \Big[\int_0^x \sigma_- e^{-\sigma_-(x-y)}\Big\{g\Big[b\phi(y,s,w_- vw) + q\eta(y,s,w_- vw) + f\psi(y,s,w_- vw)\Big] + \frac{\sigma_a}{\sigma}\delta(s)\Big\}dy + e^{-\sigma_- x}\delta(s)\Big]ds \tag{9}$$

Eqs. 7-9 state that the probability that a particle of weight w at x will contribute a score in ds about s is equal to the sum, over all possible next events, of the probability of each next event times the probability that the particle scores s in ds subsequent to the sampling of that next event. The possible next events for a particle moving in the $+\hat{x}$ direction are:

1. Collision at y with $T \geq y \geq x$, then survival at y, and then scattering in the $+\hat{x}$ direction.
2. Collision at y with $T \geq y \geq x$, then survival at y, and then scattering in the $-\hat{x}$ direction.
3. Collision at y with $T \geq y \geq x$, then survival at y, and then scattering perpendicular to the $\hat{x}$ direction.
4. Collision at y with $T \geq y \geq x$, then absorption at y.
5. Free-flight to $x = T$ and penetration of the slab.

The corresponding next event probabilities are:

1. $\sigma_+ e^{-\sigma_+(y-x)}, g, f$.
2. $\sigma_+ e^{-\sigma_+(y-x)}, g, b$.
3. $\sigma_+ e^{-\sigma_+(y-x)}, g, q$.
4. $\sigma_+ e^{-\sigma_+(y-x)}, 1-g$.
5. $e^{-\sigma_+(T-x)}$.

The probabilities that a score s in ds will subsequently occur after the above events are:

1. $\phi(y, s, w_{+}vw)ds$
2. $\psi(y, s, w_{+}vw)ds$
3. $\eta(y, s, w_{+}vw)ds$
4. $\delta(s)ds$
5. $\delta(s - ww_T)ds$

Summing the above probabilities over all next events yields Eq. 7.

Similarly, the possible next events for a particle moving in the $-\hat{x}$ direction are:

1. Collision at y with $x \geq y \geq 0$, then survival at y, and then scattering in the $+\hat{x}$ direction.
2. Collision at y with $x \geq y \geq 0$, then survival at y, and then scattering in the $-\hat{x}$ direction.
3. Collision at y with $x \geq y \geq 0$, then survival at y, and then scattering perpendicular to the $\hat{x}$ direction.
4. Collision at y with $x \geq y \geq 0$, then absorption at y.
5. Free-flight to $x = 0$.

The corresponding next event probabilities are:

1. $\sigma_{-}e^{-\sigma_{-}(x-y)}, g, b$.
2. $\sigma_{-}e^{-\sigma_{-}(x-y)}, g, f$.
3. $\sigma_{-}e^{-\sigma_{-}(x-y)}, g, q$.
4. $\sigma_{-}e^{-\sigma_{-}(x-y)}, 1 - g$.
5. $e^{-\sigma_{-}x}$.

The probabilities that a score s in ds will subsequently occur for the above events are:

1. $\phi(y, s, w_{-}vw)ds$
2. $\psi(y, s, w_{-}vw)ds$
3. $\eta(y, s, w_{-}vw)ds$
4. $\delta(s)ds$
5. $\delta(s)ds$

Summing the above probabilities over all next events yields Eq. 9.

Note that x will not change for a particle moving perpendicular to $\hat{x}$. The particle *will* collide at x and either be absorbed or scattered. Note that a forward or backward scattering still leaves the particle traveling perpendicular to $\hat{x}$, and a 90 degree scattering puts the particle in the $\pm\hat{x}$ directions with equal probabilities of $\frac{1}{2}$. The possible next events for a particle moving perpendicular to $\hat{x}$ are:

1. Collision at x, then survival, and then scattering perpendicular to the $\hat{x}$ direction.
2. Collision at x, then survival, and then scattering in the $+\hat{x}$ direction.
3. Collision at x, then survival, and then scattering in the $-\hat{x}$ direction.
4. Collision at x, then absorption.

The corresponding next event probabilities are:

1. $1, g, (f + b)$
2. $1, g, \frac{g}{2}$
3. $1, g, \frac{g}{2}$
4. $1, 1 - g$

The probabilities that a score s in ds will subsequently occur for the above events are:

1. $\eta(x, s, w_0 v w)ds$
2. $\phi(x, s, w_0 v w)ds$
3. $\psi(x, s, w_0 v w)ds$
4. $\delta(s)ds$

Because there are no weight-dependent games, a particle of weight w will have exactly the same random walk as a particle of unit weight and its tally will be w times as much. Expressed mathematically:

$$\phi(x, s, w)ds = \phi(x, \frac{s}{w}, 1)d\frac{s}{w} \doteq \phi(x, \frac{s}{w})d\frac{s}{w} \qquad (10)$$

$$\psi(x, s, w)ds = \psi(x, \frac{s}{w}, 1)d\frac{s}{w} \doteq \psi(x, \frac{s}{w})d\frac{s}{w} \qquad (11)$$

$$\eta(x, s, w)ds = \eta(x, \frac{s}{w}, 1)d\frac{s}{w} \doteq \eta(x, \frac{s}{w})d\frac{s}{w} \qquad (12)$$

where the last equality in the equations defines $\phi(x,t), \psi(x,t)$, and $\eta(x,t)$. Note that $\phi(x,t)$, $\psi(x,t)$, and $\eta(x,t)$ are the probability densities for obtaining a score t from a unit weight particle. Substituting Eqs. 10-12 into Eqs. 7-9 and letting $t = \frac{s}{w}$ yields

$$\phi(x,t)dt = \Big[\int_x^T \sigma_+ e^{-\sigma_+(y-x)}\Big\{\frac{g}{w_+vw}\Big[f\phi(y,\frac{t}{w_+v}) + q\eta(y,\frac{t}{w_+v}) + b\psi(y,\frac{t}{w_+v})\Big]$$
$$+ \frac{\sigma_a}{\sigma}\delta(wt)\Big\}dy + e^{-\sigma_+(T-x)}\delta(wt - ww_T)\Big] wdt \qquad (13)$$

$$\eta(x,t)dt = \int_0^\infty \sigma_0 e^{-\sigma_0 z}\Big\{\frac{g}{w_0vw}[\frac{q}{2}\phi(x,\frac{t}{v}) + (f+b)\eta(x,\frac{t}{v}) + \frac{q}{2}\psi(x,\frac{t}{v})] + \frac{\sigma_a}{\sigma}\delta(t)\Big\}dzwdt \qquad (14)$$

$$\psi(x,t)dt = \Big[\int_0^x \sigma_- e^{-\sigma_-(x-y)}\Big\{\frac{g}{w_-vw}\Big[b\phi(y,\frac{t}{w_-v}) + q\eta(y,\frac{t}{w_-v}) + f\psi(y,\frac{t}{w_-v})\Big]$$
$$+ \frac{\sigma_a}{\sigma}\delta(wt)\Big\}dy + e^{-\sigma_- x}\delta(wt)\Big] wdt \qquad (15)$$

Recalling that

$$\delta(ax) = \frac{1}{a}\delta(x) \qquad (16)$$

Eqs. 13 and 15 become

$$\phi(x,t)dt = \Big[\int_x^T \sigma_+ e^{-\sigma_+(y-x)}\Big\{\frac{g}{w_+v}\Big[f\phi(y,\frac{t}{w_+v}) + q\eta(y,\frac{t}{w_+v}) + b\psi(y,\frac{t}{w_+v})\Big]$$
$$+ \frac{\sigma_a}{\sigma}\delta(t)\Big\}dy + e^{-\sigma_+(T-x)}\delta(t - w_T)\Big] dt \qquad (17)$$

$$\eta(x,t)dt = \int_0^\infty \sigma_0 e^{-\sigma_0 z}\Big\{\frac{g}{w_0v}[\frac{q}{2}\phi(x,\frac{t}{v}) + (f+b)\eta(x,\frac{t}{v}) + \frac{q}{2}\psi(x,\frac{t}{v})] + \frac{\sigma_a}{\sigma}\delta(t)\Big\}dzdt \qquad (17.1)$$

$$\psi(x,t)dt = \Big[\int_0^x \sigma_- e^{-\sigma_-(x-y)}\Big\{\frac{g}{w_-v}\Big[b\phi(y,\frac{t}{w_-v}) + q\eta(y,\frac{t}{w_-v}) + f\psi(y,\frac{t}{w_-v})\Big]$$
$$+ \frac{\sigma_a}{\sigma}\delta(t)\Big\}dy + e^{-\sigma_- x}\delta(t)\Big] dt \qquad (18)$$

Define

$$L_r(x) = \int \psi(x,s)s^r ds \qquad (19)$$

$$M_r(x) = \int \eta(x,s)s^r ds \tag{20}$$

$$N_r(x) = \int \phi(x,s)s^r ds \tag{21}$$

Note that with $s = \frac{t}{wv}$

$$\int \frac{1}{wv}\phi(y,\frac{t}{wv})t^r dt = \int \frac{1}{wv}\phi(y,s)(wvs)^r d(wvs) = (wv)^r \int \phi(y,s)s^r ds = (wv)^r L_r(y) \tag{22}$$

$$\int \frac{1}{wv}\eta(y,\frac{t}{wv})t^r dt = \int \frac{1}{wv}\eta(y,s)(wvs)^r d(wvs) = (wv)^r M_r(y) \tag{23}$$

$$\int \frac{1}{wv}\psi(y,\frac{t}{wv})t^r dt = \int \frac{1}{wv}\psi(y,s)(wvs)^r d(wvs) = (wv)^r N_r(y) \tag{24}$$

Multiplying Eqs. 17.1 and 18 by t^r and integrating and using Eqs. 22-24 yields

$$L_r(x) = \int_0^x \sigma_- e^{-\sigma_-(x-y)}(vw_-)^r g\Big[bN_r(y) + qM_r(y) + fL_r(y)\Big]dy \tag{25}$$

$$M_r(x) = \int_0^\infty \sigma_0 e^{-\sigma_0 z}\Big\{(vw_0)^r g[\frac{q}{2}N_r(x) + (f+b)M_r(x) + \frac{q}{2}L_r(x)]\Big\}dz \tag{25.1}$$

Using Eq. 5.1

$$M_r(x) = v^r g[\frac{q}{2}N_r(x) + (f+b)M_r(x) + \frac{q}{2}L_r(x)] \int_0^\infty \sigma_0 e^{-\sigma_0 z}\Big\{\frac{\sigma e^{-\sigma z}}{\sigma_0 e^{-\sigma_0 z}}\Big\}^r dz \tag{25.2}$$

$$M_r(x) = v^r g[\frac{q}{2}N_r(x) + (f+b)M_r(x) + \frac{q}{2}L_r(x)]\sigma_0\{\frac{\sigma}{\sigma_0}\}^r[\sigma_0 + r(\sigma - \sigma_0)]^{-1} \tag{25.3}$$

Defining

$$G = v^r g\sigma_0\{\frac{\sigma}{\sigma_0}\}^r[\sigma_0 + r(\sigma - \sigma_0)]^{-1} \tag{25.4}$$

Eq. 25.3 becomes

$$M_r(x) = G[\frac{q}{2}N_r(x) + (f+b)M_r(x) + \frac{q}{2}L_r(x)] \tag{26}$$

Multiplying Eq. 17 by t^r, integrating, and using Eqs. 22-24 yields

$$N_r(x) = \int_x^T \sigma_+ e^{-\sigma_+(y-x)}(vw_+)^r g\Big[fN_r(y) + qM_r(y) + bL_r(y)\Big]dy + e^{-\sigma_+(T-x)}w_T^r \tag{27}$$

Using Eqs. 4-6, note that the three equations above are independent of σ_+, σ_0, and σ_- for $r = 1$. Thus the mean score is the same as the analog case for any choices of σ_+, σ_0, and σ_-; thus the method is unbiased.

Substituting Eqs. 1,2,4,5, and 6 into Eqs. 25 and 27 yields

$$L_r(x) = \int_0^x \sigma_- e^{-\sigma_-(x-y)}(\frac{\sigma}{\sigma_-})^r e^{-(\sigma-\sigma_-)(x-y)r} gv^r\Big[bN_r(y) + qM_r(y) + fL_r(y)\Big]dy \tag{28}$$

$$N_r(x) = \int_x^T \sigma_+ e^{-\sigma_+(y-x)}(\frac{\sigma}{\sigma_+})^r e^{-(\sigma-\sigma_+)(y-x)r} gv^r\Big[fN_r(y) + qM_r(y) + bL_r(y)\Big]dy + e^{-\sigma_+(T-x)}e^{-\sigma_+(T-x)r} \tag{29}$$

Rearranging the two equations above yields

$$L_r(x) = (\frac{\sigma_-}{\sigma})^{-r+1} g\sigma v^r \int_0^x e^{-(\sigma r-\sigma_-(r-1))(x-y)}\Big[bN_r(y) + qM_r(y) + fL_r(y)\Big]dy \tag{30}$$

$$N_r(x) = (\frac{\sigma_+}{\sigma})^{-r+1} g\sigma v^r \int_x^T e^{-(\sigma r-\sigma_+(r-1))(y-x)}\Big[fN_r(y) + qM_r(y) + bL_r(y)\Big]dy + e^{-(\sigma r-\sigma_+(r-1))(T-x)} \tag{31}$$

Multiplying Eq. 30 by $e^{(\sigma r-\sigma_-(r-1))x}$ and Eq. 31 by $e^{-(\sigma r-\sigma_+(r-1))x}$ yields

$$L_r(x)e^{(\sigma r-\sigma_-(r-1))x} = (\frac{\sigma_-}{\sigma})^{-r+1} g\sigma v^r \int_0^x e^{(\sigma r-\sigma_-(r-1))y}\Big[bN_r(y)+qM_r(y)+fL_r(y)\Big]dy \tag{32}$$

$$N_r(x)e^{-(\sigma r-\sigma_+(r-1))x} = (\frac{\sigma_+}{\sigma})^{-r+1} g\sigma v^r \int_x^T e^{-(\sigma r-\sigma_+(r-1))y}\Big[fN_r(y)+qM_r(y)+bL_r(y)\Big]dy$$
$$+\,e^{-(\sigma r-\sigma_+(r-1))T} \tag{33}$$

Differentiating Eqs. 32 and 33 yields

$$L_r'(x)e^{(\sigma r-\sigma_-(r-1))x} + (\sigma r-\sigma_-(r-1))L_r(x)e^{(\sigma r-\sigma_-(r-1))x}$$
$$= (\frac{\sigma_-}{\sigma})^{-r+1}\sigma g v^r e^{(\sigma r-\sigma_-(r-1))x} \tag{34}$$
$$\times \Big[bN_r(x)+qM_r(x)+fL_r(x)\Big]$$

$$N_r'(x)e^{-(\sigma r-\sigma_+(r-1))x} - (\sigma r-\sigma_+(r-1))N_r(x)e^{-(\sigma r-\sigma_+(r-1))x}$$
$$= -(\frac{\sigma_+}{\sigma})^{-r+1}\sigma g v^r e^{-(\sigma r-\sigma_+(r-1))x} \tag{35}$$
$$\times \Big[fN_r(x)+qM_r(x)+bL_r(x)\Big]$$

Multiplying Eqs. 34 and 35 by $e^{-(\sigma r-\sigma_-(r-1))x}$ and $e^{(\sigma r-\sigma_+(r-1))x}$ respectively yields

$$L_r'(x) + (\sigma r-\sigma_-(r-1))L_r(x) = (\frac{\sigma_-}{\sigma})^{-r+1}\sigma g v^r\Big[bN_r(x)+qM_r(x)+fL_r(x)\Big] \tag{36}$$

$$N_r'(x) - (\sigma r-\sigma_+(r-1))N_r(x) = -(\frac{\sigma_+}{\sigma})^{-r+1}\sigma g v^r\Big[fN_r(x)+qM_r(x)+bL_r(x)\Big] \tag{37}$$

Rearranging Eq. 26 and defining D by

$$D = \frac{q^2}{2}\frac{G}{1-G(f+b)} \tag{37.1}$$

yields

$$M_r(x) = \frac{D}{q}(N_r(x)+L_r(x)) \tag{38}$$

Substituting Eq. 38 into Eqs. 36 and 37 yields

$$L_r'(x)+(\sigma r-\sigma_-(r-1))L_r(x) = (\frac{\sigma_-}{\sigma})^{-r+1}\sigma g v^r\left[bN_r(x)+D(N_r(x)+L_r(x))+fL_r(x)\right] \quad (39)$$

$$N_r'(x) - (\sigma r - \sigma_+(r-1))N_r(x) = -(\frac{\sigma_+}{\sigma})^{-r+1}\sigma g v^r\left[fN_r(x) + D(N_r(x) + L_r(x)) + bL_r(x)\right] \quad (40)$$

Rearranging yields

$$L_r'(x)+\left[(\sigma r-\sigma_-(r-1))-(\frac{\sigma_-}{\sigma})^{-r+1}\sigma g v^r(D+f)\right]L_r(x) = (\frac{\sigma_-}{\sigma})^{-r+1}\sigma g v^r\left[b+D\right]N_r(x) \quad (41)$$

$$\begin{aligned} N_r'(x) + &\left[(\frac{\sigma_+}{\sigma})^{-r+1}\sigma g v^r(f + D) - (\sigma r - \sigma_+(r-1))\right]N_r(x) \\ &= -(\frac{\sigma_+}{\sigma})^{-r+1}\sigma g v^r\left[D + b\right]L_r(x) \end{aligned} \quad (42)$$

Defining

$$\alpha = \left[(\frac{\sigma_+}{\sigma})^{-r+1}\sigma g v^r(f + D) - (\sigma r - \sigma_+(r-1))\right] \quad (43)$$

$$\beta = -(\frac{\sigma_+}{\sigma})^{-r+1}\sigma g v^r\left[D + b\right] \quad (44)$$

$$\gamma = \left[(\sigma r - \sigma_-(r-1)) - (\frac{\sigma_-}{\sigma})^{-r+1}\sigma g v^r(D + f)\right] \quad (45)$$

$$\epsilon = (\frac{\sigma_-}{\sigma})^{-r+1}\sigma g v^r\left[b + D\right] \quad (46)$$

and inserting into Eqs. 41 and 42 yields

$$L_r'(x) + \gamma L_r(x) = \epsilon N_r(x) \quad (47)$$

$$N_r'(x) + \alpha N_r(x) = \beta L_r(x) \quad (48)$$

This is a system of first order linear differential equations so one tries a solution of the form[7]:

$$N_r(x) = ae^{r_1 x} + be^{r_2 x} \tag{49}$$

$$L_r(x) = ce^{r_1 x} + de^{r_2 x} \tag{50}$$

A particle at $x = 0$ moving backwards always scores 0 thus,

$$L_r(0) = 0. \tag{51}$$

Applying this boundary condition yields $d = -c$ so that

$$L_r(x) = c(e^{r_1 x} - e^{r_2 x}) \tag{52}$$

Substituting Eqs. 49 and 52 into Eqs. 47 and 48 yields

$$ar_1 e^{r_1 x} + br_2 e^{r_2 x} + a\alpha e^{r_1 x} + b\alpha e^{r_2 x} = \beta c(e^{r_1 x} - e^{r_2 x}) \tag{53}$$

$$r_1 ce^{r_1 x} - cr_2 e^{r_2 x} + \gamma c(e^{r_1 x} - e^{r_2 x}) = \epsilon ae^{r_1 x} + \epsilon be^{r_2 x} \tag{54}$$

Collecting coefficients of the exponentials in Eqs. 53 and 54 yields

$$a(r_1 + \alpha) = \beta c \tag{55}$$

$$b(r_2 + \alpha) = -\beta c \tag{56}$$

$$c(r_1 + \gamma) = \epsilon a \tag{57}$$

$$-c(r_2 + \gamma) = \epsilon b \tag{58}$$

Solving Eqs. 55 and 57 together and Eqs. 56 and 58 together yields

$$r_1^2 + (\alpha + \gamma)r_1 + (\alpha\gamma - \beta\epsilon) = 0 \tag{59}$$

$$r_2^2 + (\alpha + \gamma)r_2 + (\alpha\gamma - \beta\epsilon) = 0 \tag{60}$$

Eqs. 59 and 60 are the same, so take

$$r_1 = \frac{1}{2}\Big[-(\alpha+\gamma) - \sqrt{(\alpha+\gamma)^2 - 4(\alpha\gamma - \beta\epsilon)}\Big] = \frac{1}{2}\Big[-(\alpha+\gamma) - \sqrt{(\alpha-\gamma)^2 + 4\beta\epsilon}\Big] \quad (61)$$

$$r_2 = \frac{1}{2}\Big[-(\alpha+\gamma) + \sqrt{(\alpha+\gamma)^2 - 4(\alpha\gamma - \beta\epsilon)}\Big] = \frac{1}{2}\Big[-(\alpha+\gamma) + \sqrt{(\alpha-\gamma)^2 + 4\beta\epsilon}\Big] \quad (62)$$

A particle at $x = T$ moving in the $+\hat{x}$ direction always scores exactly 1, so that

$$N_r(T) = 1 \quad (63)$$

From Eqs. 57 and 58

$$a = -b\frac{r_1+\gamma}{r_2+\gamma} \quad (64)$$

Using Eqs. 49 (at $x = T$),63, and 64 yields

$$1 = -b\frac{r_1+\gamma}{r_2+\gamma}e^{r_1 T} + be^{r_2 T} \quad (65)$$

Solving for b yields

$$b = \Big[e^{r_2 T} - \frac{r_1+\gamma}{r_2+\gamma}e^{r_1 T}\Big]^{-1} \quad (66)$$

Substituting Eqs. 66 and 64 into Eq. 49 yields

$$N_r(x) = \Big[e^{r_2 T} - \frac{r_1+\gamma}{r_2+\gamma}e^{r_1 T}\Big]^{-1}\Big[-\frac{r_1+\gamma}{r_2+\gamma}e^{r_1 x} + e^{r_2 x}\Big] \quad (67)$$

Multiplying the numerator and denominator of Eq. 67 by $r_2 + \gamma$ yields

$$N_r(x) = \Big[-(r_1+\gamma)e^{r_1 x} + (r_2+\gamma)e^{r_2 x}\Big]\Big[-(r_1+\gamma)e^{r_1 T} + e^{r_2 T}(r_2+\gamma)\Big]^{-1} \quad (68)$$

Note from Eq. 68 that the r^{th} moment becomes infinite when the denominator vanishes; that is, when

$$T_c = \frac{1}{r_2 - r_1} ln\Big[\frac{r_1+\gamma}{r_2+\gamma}\Big] \quad (69)$$

Consider the case when r_1 and r_2 are complex. Note that the imaginary parts of r_1 and r_2 are the same magnitudes but opposite signs; thus define z and y by

$$r_1 \doteq z - iy \tag{70}$$

$$r_2 \doteq z + iy \tag{71}$$

Additionally define θ and ρ by,

$$r_1 + \gamma = \rho e^{-i\theta} \tag{72}$$

$$r_2 + \gamma = \rho e^{i\theta} \tag{73}$$

Substituting into Eq. 69 yields

$$T_c = \frac{1}{i2y} ln\left[\frac{\rho e^{-i\theta}}{\rho e^{i\theta}}\right] \tag{74}$$

or

$$T_c = \frac{1}{i2y} ln\left[e^{-i2\theta}\right] \tag{75}$$

Recalling that (for integer m) $e^{i(\phi+2\pi m)} = e^{i\phi}$,

$$T_c = \frac{1}{y}\left[m\pi - arctan\left[\frac{y}{z+\gamma}\right]\right] \tag{76}$$

Note that for complex roots that there is *always* a positive solution for T_c for some m. For practical purposes, the smallest positive T_c is the one of interest. A computer program to calculate critical thickness is given in Appendix A together with a specific example.

Rewriting the numerator of Eq. 68 using Eqs. 70 and 71 yields

$$-(r_1 + \gamma)e^{r_1 x} + (r_2 + \gamma)e^{r_2 x} = -(z - iy + \gamma)e^{(z-iy)x} + (z + iy + \gamma)e^{(z+iy)x} \tag{77}$$

$$= e^{zx}\{(z+\gamma)e^{iyx} - (z+\gamma)e^{-iyx} + iy(e^{iyx} + e^{-iyx})\} = 2ie^{zx}\{(z+\gamma)sin(yx) + ycos(yx)\} \tag{78}$$

Note that the denominator of Eq. 68 is the same as the numerator evaluated at $x = T$, thus

$$N_r(x) = \left[e^{zx}\{(z+\gamma)sin(yx) + ycos(yx)\}\right]\left[e^{zT}\{(z+\gamma)sin(yT) + ycos(yT)\}\right]^{-1} \quad (79)$$

A computer program that calculates the moments from Eq. 79 and estimates the moments via Monte Carlo transport is given in Appendix B together with a specific example.

IV. DERIVATION OF SCORE DISTRIBUTION EQUATIONS

The moment equations of the previous section allow determination of the critical thickness for a slab with given $\sigma, \sigma_s, \sigma_+, \sigma_0$, and σ_-, but the actual score distribution is also interesting. The special case for which:

$$\sigma_+ = \sigma(1-p) \quad (79.1)$$

$$\sigma_0 = \sigma \quad (79.2)$$

$$\sigma_- = \sigma(1+p) \quad (79.3)$$

will now be considered because it is the tridirectional analog of the oldest exponential transform variation in MCNP.

It will be shown that the score distribution (for the choices Eqs. 79.1-79.3) is a discrete distribution, determined *only* by the number of collisions the particle has while moving in the forward direction and the number of collisions the particle has while moving in the backward direction. Most of the theory for this comes directly from the MCNP manual (ref. 1, p. 144), and is paraphrased in the next paragraph.

Consider the penetration of a nonmultiplying slab whose nuclear cross sections are constants, independent of space and energy. Let the desired tally be a simple count of the number of neutrons penetrating the slab per incident source neutron. Consider artificially changing the total cross section from σ to $\sigma' = \sigma(1 - p\mu)$ where μ is the cosine with respect to the slab penetration direction and p is the transform parameter. The weight multiplication upon collision is

$$w_c = \frac{e^{-p\sigma\mu s}}{1 - p\mu}, \tag{80}$$

where s is the sampled distance traveled by the particle for the current sampling. If the particle does not collide because it reaches a geometric surface before collision, then the weight multiplication is

$$w_s = e^{-p\sigma\mu s} \tag{81}$$

Suppose for a given penetrating particle that there are k flights, m that collide and $k - m$ that do not collide. (Note that there may be many geometric surfaces in the slab for such things as tallying even though the slab is homogeneous, thus there may be many collisionless flights.) The penetrating weight is:

$$w_p = \prod_{i=1}^{m} \frac{e^{-p\sigma\mu_i s_i}}{1 - p\mu_i} \prod_{j=m+1}^{k} e^{-p\sigma\mu_j s_j} \tag{82}$$

However, note that the particle's penetration of a slab of thickness T means that

$$\sum_{l=1}^{k} \mu_l s_l = T \tag{83}$$

and hence

$$w_p = e^{-p\sigma T} \prod_{i=1}^{m} (1 - p\mu_i)^{-1} \tag{84}$$

Note that the only variation in w_p is because of the $(1 - p\mu_i)^{-1}$ factors that arise from collisions. *Every* particle that penetrates has the *same* exponential factor $e^{-p\sigma T}$ regardless of how it penetrates the slab. Thus the variation in weight is due to the number and type of collisions; that is, how many collisions of positive μ and how many of negative μ.

Now consider a problem with only three possible directions; that is $\mu_i = \{-1, 0, 1\}$. Using Eqs. 79.1-79.3 in Eq. 84 to obtain the penetrating weight, and hence the scores, yields

$$s_{mn} = (1 - p)^{-m}(1 + p)^{-n} e^{-p\sigma T} v^{m+n} \quad , \tag{85}$$

where m is the number of collisions in the forward direction and n is the number of collisions in the backward direction. This is a discrete score distribution and all that is now lacking are the probabilities of having m collisions in the forward direction and n collisions in the backward direction. Define

Definition 7. $\phi_{mn}(x) =$ the probability that a particle moving in the forward direction will penetrate the slab after making *exactly* m collisions while moving in the forward direction and *exactly* n collisions while moving in the backward direction.

Definition 8. $\eta_{mn}(x) =$ the probability that a particle moving in the perpendicular direction will penetrate the slab after making *exactly* m collisions while moving in the forward direction and *exactly* n collisions while moving in the backward direction.

Definition 9. $\phi_{mn}(x) =$ the probability that a particle moving in the backward direction will penetrate the slab after making *exactly* m collisions while moving in the forward direction and *exactly* n collisions while moving in the backward direction.

Following the earlier procedure, the equations for $\phi_{mn}(x)$, $\eta_{mn}(x)$, and $\psi_{mn}(x)$ are written and then explained below.

$$\phi_{mn}(x) = \int_x^T \sigma_+ e^{-\sigma_+(y-x)} g\Big[f\phi_{m-1,n}(y) + q\eta_{m-1,n}(y) + b\psi_{m-1,n}(y)\Big]dy \qquad m \geq 1 \quad (86)$$

$$\eta_{mn}(x) = g\Big[\frac{q}{2}\phi_{mn}(x) + \frac{q}{2}\psi_{mn}(x) + (f+b)\eta_{mn}(x)\Big] \quad (87)$$

$$\psi_{mn}(x) = \int_0^x \sigma_- e^{-\sigma_-(x-y)} g\Big[b\phi_{m,n-1}(y) + q\eta_{m,n-1}(y) + f\psi_{m,n-1}(y)\Big]dy \qquad n \geq 1 \quad (88)$$

Equation 86 states that the probability that a particle makes exactly $m \geq 1$ collisions in the forward direction and exactly $n \geq 0$ collisions in the backward direction is equal to the probability of each next event, times the probability (subsequent to that next event) that the correct number of collisions occur in the two directions. The possible next events for a particle moving in the $+\hat{x}$ direction are:

1. Collision at y with $T \geq y \geq x$, then survival at y, and then scattering in the $+\hat{x}$ direction.
2. Collision at y with $T \geq y \geq x$, then survival at y, and then scattering in the $-\hat{x}$ direction.
3. Collision at y with $T \geq y \geq x$, then survival at y, and then scattering in the direction perpendicular to $\hat{x}$.
4. Collision at y with $T \geq y \geq x$, then absorption at y.
5. Free-flight to $x = T$ and penetration of the slab.

The corresponding next event probabilities are:

1. $\sigma_+ e^{-\sigma_+(y-x)}, g, f$.
2. $\sigma_+ e^{-\sigma_+(y-x)}, g, b$.
3. $\sigma_+ e^{-\sigma_+(y-x)}, g, q$.
4. $\sigma_+ e^{-\sigma_+(y-x)}, 1 - g$.
5. $e^{-\sigma_+(T-x)}$.

The probabilities (subsequent to each of the above events) that the sum of the collisions for a *penetrating* particle will be m, n are:

1. $\phi_{m-1,n}(y)$
2. $\psi_{m-1,n}(y)$
3. $\eta_{m-1,n}(y)$
4. 0
5. 0

The probability in 4 is zero because an absorbed particle cannot penetrate; the probability in 5 is zero because a free-flight leads to $m = 0$ and Eq. 86 requires at least one collision. Summing the above probabilities over all next events yields Eq. 86.

The possible next events for a particle moving perpendicular to $\hat{x}$ are

1. Collision at x, then survival, and then scattering in the $+\hat{x}$ direction.
2. Collision at x, then survival, and then scattering in the $-\hat{x}$ direction.
3. Collision at x, then survival, and then scattering in the direction perpendicular to $\hat{x}$.
4. Collision at x, then absorption at x.

The corresponding next event probabilities are:

1. $1, g, \frac{q}{2}$.
2. $1, g, \frac{q}{2}$.
3. $1, g, f + b$.
4. $1, 1 - g$.

The probabilities (subsequent to each of the above events) that the sum of the collisions for a *penetrating* particle will be m, n are:

1. $\phi_{mn}(x)$
2. $\psi_{mn}(x)$
3. $\eta_{mn}(x)$
4. 0

Summing the above probabilities over all next events yields Eq. 87.

The possible next events for a particle moving in the $-\hat{x}$ direction are:

1. Collision at y with $x \geq y \geq 0$, then survival at y, and then scattering in the $+\hat{x}$ direction.
2. Collision at y with $x \geq y \geq 0$, then survival at y, and then scattering in the $-\hat{x}$ direction.
3. Collision at y with $x \geq y \geq 0$, then survival at y, and then scattering perpendicular to the $\hat{x}$.
4. Collision at y with $x \geq y \geq 0$, then absorption at y.
5. Free-flight to $x = 0$.

The corresponding next event probabilities are:

1. $\sigma_- e^{-\sigma_-(x-y)}, g, b$.
2. $\sigma_- e^{-\sigma_-(x-y)}, g, f$.
3. $\sigma_- e^{-\sigma_-(x-y)}, g, q$.
4. $\sigma_- e^{-\sigma_-(x-y)}, 1 - g$.
5. $e^{-\sigma_- x}$.

The probabilities (subsequent to each of the above events) that the sum of the collisions for a penetrating particle will be m, n are:

1. $\phi_{m,n-1}(y)$
2. $\psi_{m,n-1}(y)$
3. $\eta_{m,n-1}(y)$
4. 0
5. 0

Note that the probabilities in 4 and 5 are 0 because a particle cannot penetrate ($x = T$) if it is absorbed nor if it crosses $x = 0$. Summing the above probabilities over all next events yields Eq. 88.

Rearranging Eq. 87 and defining

$$Q = gq^2[1 - (f + b)g]^{-1} \tag{89}$$

yields

$$\eta_{mn}(x) = \frac{Q}{2}[\phi_{mn} + \psi_{mn}] \tag{90}$$

Substituting Eq. 90 into Eqs. 86 and 88 yields

$$\phi_{mn}(x) = \int_x^T \sigma_+ e^{-\sigma_+(y-x)} g\left[(f + \frac{Q}{2})\phi_{m-1,n}(y) + (b + \frac{Q}{2})\psi_{m-1,n}(y)\right] dy \qquad m \geq 1 \tag{91}$$

$$\psi_{mn}(x) = \int_0^x \sigma_- e^{-\sigma_-(x-y)} g\left[(b + \frac{Q}{2})\phi_{m,n-1}(y) + (f + \frac{Q}{2})\psi_{m,n-1}(y)\right] dy \qquad n \geq 1 \tag{92}$$

Rewrite Eqs. 91 and 92 in terms of the distance from the $x = T$ boundary. That is, let

$$s = T - x \tag{93}$$

$$F_{mn}(s) = \phi_{mn}(x) \tag{94}$$

$$B_{mn}(s) = \psi_{mn}(x) \tag{95}$$

Additionally, let

$$K = \frac{g\sigma_+}{2} \tag{96}$$

$$M = \frac{g\sigma_-}{2} \tag{97}$$

$$r = T - y \tag{98}$$

$$\alpha = 2f + Q \tag{99}$$

$$\beta = 2b + Q \tag{100}$$

Changing variables from x and y to s and r yields

$$F_{mn}(s) = Ke^{-\sigma_+ s} \int_0^s e^{\sigma_+ r} \left[(\alpha F_{m-1n}(r) + \beta B_{m-1n}(r) \right] dr \tag{101}$$

$$B_{mn}(s) = Me^{\sigma_- s} \int_s^T e^{-\sigma_- r} \left[(\beta F_{mn-1}(r) + \alpha B_{mn-1}(r) \right] dr \tag{102}$$

Note that

$$B_{m0}(s) = 0 \qquad for \qquad m \geq 0 \tag{103}$$

because a particle moving in the backward direction that does not have at least one collision while moving backward cannot penetrate the slab. Also, note that

$$F_{0n}(s) = 0 \qquad for \qquad n > 0 \tag{104}$$

because a particle moving forward cannot have any collisions moving backward if there are no collisions while moving forward. Finally, a collisionless free-flight that penetrates the slab occurs with probability

$$F_{00}(x) = e^{-\sigma_+ s} \tag{105}$$

After evaluating the solutions for small m, n it appears that good guesses for B_{mn} and F_{mn} are:

$$F_{mn}(s) = e^{-\sigma_+ s}\sum_{j=0}^{m} a_{mnj}s^j + e^{\sigma_- s}\sum_{j=0}^{n-1} b_{mnj}s^j \tag{106}$$

$$B_{mn}(s) = e^{-\sigma_+ s}\sum_{j=0}^{m} c_{mnj}s^j + e^{\sigma_- s}\sum_{j=0}^{n-1} d_{mnj}s^j \tag{107}$$

From integral tables for positive integers n

$$\int x^n e^{ax}dx = \frac{e^{ax}}{a^{n+1}}\sum_{k=0}^{n}(-1)^{n+k}\frac{n!}{k!}(ax)^k \tag{108}$$

Substituting Eqs. 106 and 107 into Eqs. 101 and 102 yields

$$\begin{aligned} F_{mn}(s) = Ke^{-\sigma_+ s}\int_0^s e^{\sigma_+ r}\Big[\alpha\{e^{-\sigma_+ r}\sum_{j=0}^{m-1} a_{m-1,nj}r^j + e^{\sigma_- r}\sum_{j=0}^{n-1} b_{m-1,nj}r^j\} \\ + \beta\{e^{-\sigma_+ r}\sum_{j=0}^{m-1} c_{m-1,nj}r^j + e^{\sigma_- r}\sum_{j=0}^{n-1} d_{m-1,nj}r^j\}\Big]dr \end{aligned} \tag{109}$$

Defining

$$\sigma_* = \sigma_+ + \sigma_- \tag{109.1}$$

$$\begin{aligned} F_{mn}(s) = Ke^{-\sigma_+ s}\int_0^s \Big[\alpha\sum_{j=0}^{m-1} a_{m-1,nj}r^j + e^{\sigma_* r}\alpha\sum_{j=0}^{n-1} b_{m-1,nj}r^j \\ + \beta\sum_{j=0}^{m-1} c_{m-1,nj}r^j + e^{\sigma_* r}\beta\sum_{j=0}^{n-1} d_{m-1,nj}r^j\Big]dr \end{aligned} \tag{110}$$

$$\begin{aligned} F_{mn}(s) = Ke^{-\sigma_+ s}\Big[\sum_{j=0}^{m-1}(\alpha a_{m-1,nj} + \beta c_{m-1,nj})\frac{r^{j+1}}{j+1}\Big|_0^s \\ + \sum_{j=0}^{n-1}(\alpha b_{m-1,nj} + \beta d_{m-1,nj})\int_0^s e^{\sigma_* r}r^j dr\Big] \end{aligned} \tag{111}$$

Let $i = j + 1$ in the first sum and use Eq. 108 on the integral

$$F_{mn}(s) = Ke^{-\sigma_*s}\Big[\sum_{i=1}^{m}(\alpha a_{m-1,n,i-1} + \beta c_{m-1,n,i-1})\frac{s^i}{i}$$

$$+ \sum_{j=0}^{n-1}(\alpha b_{m-1,nj} + \beta d_{m-1,nj})\left\{\frac{e^{\sigma_*r}}{(\sigma_*)^{j+1}}\sum_{k=0}^{j}(-1)^{j+k}\frac{j!}{k!}(\sigma_*r)^k\right\}_0^s\Big] \tag{112}$$

$$F_{mn}(s) = Ke^{-\sigma_*s}\Big[\sum_{i=1}^{m}(\alpha a_{m-1,n,i-1} + \beta c_{m-1,n,i-1})\frac{s^i}{i} + \sum_{j=0}^{n-1}(\alpha b_{m-1,nj} + \beta d_{m-1,nj})$$

$$\times\left\{\frac{e^{\sigma_*s}}{(\sigma_*)^{j+1}}\sum_{k=0}^{j}(-1)^{j+k}\frac{j!}{k!}(\sigma_*s)^k + \left[\frac{-1}{\sigma_*}\right]^{j+1}j!\right\}\Big] \tag{113}$$

Noting that

$$\sum_{j=0}^{n-1}\sum_{k=0}^{j} = \sum_{k=0}^{n-1}\sum_{j=k}^{n-1}, \tag{114}$$

the double sum term may be rewritten and Eq. 113 becomes

$$F_{mn}(s) = Ke^{-\sigma_*s}\sum_{i=1}^{m}(\alpha a_{m-1,n,i-1} + \beta c_{m-1,n,i-1})\frac{s^i}{i}$$

$$+ Ke^{\sigma-s}\sum_{k=0}^{n-1}\sum_{j=k}^{n-1}(\alpha b_{m-1,nj} + \beta d_{m-1,nj})(\sigma_*)^{k-j-1}(-1)^{j+k}\frac{j!}{k!}s^k \tag{115}$$

$$+ Ke^{-\sigma_*s}\sum_{j=0}^{n-1}(\alpha b_{m-1,nj} + \beta d_{m-1,nj})\left(\frac{-1}{\sigma_*}\right)^{j+1}j!$$

Collecting coefficients of $s^0e^{-\sigma_*s}$ yields

$$a_{mn0} = K\sum_{j=0}^{n-1}(\alpha b_{m-1,nj} + \beta d_{m-1,nj})\left[\frac{-1}{\sigma_*}\right]^{j+1}j! \tag{116}$$

Collecting coefficients of $s^je^{-\sigma_*s}$ yields

$$a_{mnj} = \frac{K}{j}\Big(\alpha a_{m-1,n,j-1} + \beta c_{m-1,n,j-1}\Big) \qquad 1 \le j \le m \tag{117}$$

Collecting coefficients of $s^k e^{\sigma - s}$ yields

$$b_{mnk} = K \sum_{j=k}^{n-1} (\alpha b_{m-1,nj} + \beta d_{m-1,nj})(\sigma_*)^{k-j-1}(-1)^{j+k}\frac{j!}{k!} \qquad 0 \le k \le n-1 \tag{118}$$

For the backward equation, substitute Eqs. 106 and 107 into Eq. 102

$$\begin{aligned} B_{mn}(s) = M e^{\sigma - s} \int_s^T e^{-\sigma - r}\Big[& e^{-\sigma + r} \sum_{j=0}^{m} \beta a_{m,n-1,j} r^j + e^{\sigma - r} \sum_{j=0}^{n-2} \beta b_{m,n-1,j} r^j \\ & + e^{-\sigma + r} \sum_{j=0}^{m} \alpha c_{m,n-1,j} r^j + e^{\sigma - r} \sum_{j=0}^{n-2} \alpha d_{m,n-1,j} r^j \Big] dr \qquad n \ge 1 \end{aligned} \tag{119}$$

$$\begin{aligned} B_{mn}(s) = M e^{\sigma - s} \int_s^T \Big[& e^{-\sigma_* r} \sum_{j=0}^{m} \beta a_{m,n-1,j} r^j + \sum_{j=0}^{n-2} \beta b_{m,n-1,j} r^j \\ & + e^{-\sigma_* r} \sum_{j=0}^{m} \alpha c_{m,n-1,j} r^j + \sum_{j=0}^{n-2} \alpha d_{m,n-1,j} r^j \Big] dr \qquad n \ge 1 \end{aligned} \tag{120}$$

$$\begin{aligned} B_{mn}(s) = M e^{\sigma - s} \Big[& \sum_{j=0}^{m} (\beta a_{m,n-1,j} + \alpha c_{m,n-1,j}) \int_s^T e^{-\sigma_* r} r^j dr \\ & + \sum_{j=0}^{n-2} (\beta b_{m,n-1,j} + \alpha d_{m,n-1,j}) \int_s^T r^j dr \Big] \qquad n \ge 1 \end{aligned} \tag{121}$$

Now using Eq. 108

$$\begin{aligned} B_{mn}(s) = M e^{\sigma - s} \Big[& \sum_{j=0}^{m} (\beta a_{m,n-1,j} + \alpha c_{m,n-1,j}) \Big\{ \frac{-e^{-\sigma_* r}}{(\sigma_*)^{j+1}} \sum_{k=0}^{j} (\sigma_* r)^k \frac{j!}{k!} \Big\}_{r=s}^{r=T} \\ & + \sum_{j=0}^{n-2} (\beta b_{m,n-1,j} + \alpha d_{m,n-1,j}) \Big\{ \frac{r^{j+1}}{j+1} \Big\}_{r=s}^{r=T} \Big] \qquad n \ge 1 \end{aligned} \tag{122}$$

$$B_{mn}(s) = Me^{\sigma - s}\Bigg[\sum_{j=0}^{m}(\beta a_{m,n-1,j} + \alpha c_{m,n-1,j})$$

$$\times \left\{\frac{e^{-\sigma_* s}}{(\sigma_*)^{j+1}}\sum_{k=0}^{j}(\sigma_*)^k\frac{j!}{k!}s^k - \frac{e^{-\sigma_* T}}{(\sigma_*)^{j+1}}\sum_{k=0}^{j}(\sigma_*)^k\frac{j!}{k!}T^k\right\} \tag{123}$$

$$+\sum_{j=0}^{n-2}(\beta b_{m,n-1,j} + \alpha d_{m,n-1,j})\left\{\frac{T^{j+1}}{j+1} - \frac{s^{j+1}}{j+1}\right\}\Bigg] \qquad n \geq 1$$

Letting $i = j + 1$ in the last sum, noting that $\sigma_* = \sigma_+ + \sigma_-$, and noting that

$$\sum_{j=0}^{m}\sum_{k=0}^{j} = \sum_{k=0}^{m}\sum_{j=k}^{m} \tag{124}$$

yields

$$B_{mn}(s) = Me^{-\sigma_+ s}\sum_{k=0}^{m}\sum_{j=k}^{m}(\beta a_{m,n-1,j} + \alpha c_{m,n-1,j})(\sigma_*)^{k-j-1}\frac{j!}{k!}s^k$$

$$- Me^{\sigma - s}e^{-\sigma_* T}\sum_{k=0}^{m}\sum_{j=k}^{m}(\beta a_{m,n-1,j} + \alpha c_{m,n-1,j})(\sigma_*)^{k-j-1}\frac{j!}{k!}T^k$$

$$+ Me^{\sigma - s}\sum_{j=0}^{n-2}(\beta b_{m,n-1,j} + \alpha d_{m,n-1,j})\frac{T^{j+1}}{j+1} \tag{125}$$

$$- Me^{\sigma - s}\sum_{i=1}^{n-1}(\beta b_{m,n-1,i-1} + \alpha d_{m,n-1,i-1})\frac{s^i}{i} \qquad n \geq 1$$

$$B_{mn}(s) = Me^{\sigma - s}\Bigg[\sum_{j=0}^{m}(\beta a_{m,n-1,j} + \alpha c_{m,n-1,j})\left\{\frac{-e^{-\sigma_* \tau}}{(\sigma_*)^{j+1}}\sum_{k=0}^{j}(\sigma_* \tau)^k\frac{j!}{k!}\right\}_{\tau=s}^{\tau=T}$$

$$+\sum_{j=0}^{n-2}(\beta b_{m,n-1,j} + \alpha d_{m,n-1,j})\left\{\frac{\tau^{j+1}}{j+1}\right\}_{\tau=s}^{\tau=T}\Bigg] \qquad n \geq 1 \tag{126}$$

Collecting terms of $s^k e^{-\sigma_+ s}$ yields

$$c_{mnk} = M\sum_{j=k}^{m}(\beta a_{m,n-1,j} + \alpha c_{m,n-1,j})(\sigma_*)^{k-j-1}\frac{j!}{k!} \qquad 0 \leq k \leq m \tag{127}$$

Collecting terms of $e^{\sigma_* - s}$ yields

$$d_{mn0} = M \sum_{j=0}^{n-2} (\beta b_{m,n-1,j} + \alpha d_{m,n-1,j}) \frac{T^{j+1}}{j+1} - M e^{-\sigma_* T} \sum_{k=0}^{m} \sum_{j=k}^{m} (\beta a_{m,n-1,j} + \alpha c_{m,n-1,j})(\sigma_*)^{k-j-1} \frac{j!}{k!} T^k \tag{128}$$

Collecting terms of $s^i e^{\sigma_* - s}$ yields

$$d_{mni} = -\frac{M}{i}(\beta b_{m,n-1,i-1} + \alpha d_{m,n-1,i-1}) \qquad 1 \le i \le n-1 \tag{129}$$

These recurrence relations may be solved recursively to obtain the exact score distribution. Although closed form solutions have been obtained for some cases, the author has been unable to obtain a general closed form solution.

One simple case can be obtained by induction. Assume that

$$F_{m0}(s) = (K\alpha)^m \frac{s^m}{m!} e^{-\sigma_* + s} \tag{130}$$

then using Eqs. 101 and 103

$$\begin{aligned} F_{m+1,0}(s) &= (K\alpha)^{m+1} e^{-\sigma_* + s} \int_0^s e^{\sigma_* + r} \frac{r^m}{m!} e^{-\sigma_* + r} dr \\ &= (K\alpha)^{m+1} e^{-\sigma_* + s} \int_0^s \frac{r^m}{m!} = (K\alpha)^{m+1} \frac{s^{m+1}}{(m+1)!} e^{-\sigma_* + s} \quad . \end{aligned} \tag{131}$$

However, note that Eq. 130 is true for $m = 0$, thus by induction it is true for all $m \ge 0$. Thus by Eqs. 106 and 130

$$a_{m0j} = \frac{(K\alpha)^m}{m!} \delta_{mj} \quad \textit{for } m \ge 0 \tag{132}$$

V. EXPONENTIAL TRANSFORM WITH IMPLICIT CAPTURE

The exponential transform can be used with implicit capture. The implicit capture technique splits the colliding particle into its absorbed and surviving components. That is, if the capture probability is c, then a colliding particle of weight w

has weight cw absorbed at the collision and weight $(1-c)w$ that survives and continues its transport. For the case of exponential transform with implicit capture, the definitions of v and g are changed from their definitions in Eqs. 6.4 and 6.5 to:

$$v = \frac{\sigma_s}{\sigma} \tag{133}$$

$$g = 1 \tag{134}$$

That is, v is the weight change due to the capture game, and g is the probability the particle survives the collision. For implicit capture, the particle continues its random walk with probability $g = 1$, and there is a weight change so that $v = \frac{\sigma_s}{\sigma}$. In addition, Eq. 85 includes the effect of implicit captures on the scoring weight through the v^{m+n} term. A computer program that recursively solves for a_{mnj}, b_{mnj}, c_{mnj}, and d_{mnj} is given in Appendix C. Additionally, therein lies a specific comparison of the theoretical score probability function F_{mn} with an empirical score probability function estimated by a Monte Carlo transport calculation.

VI. CONCLUSION

This report provides analytic score distributions and moments for an interesting set of spatially continuous exponential transform problems. These analytic score distributions are intended to aid in the quest for better Monte Carlo confidence statements. Proposed new confidence interval estimation procedures can use the known score distributions as test cases.

ACKNOWLEDGMENTS

I would like to thank R. A. Forster, John S. Hendricks, and Shane P. Pederson for useful discussions concerning the implications of the theory discussed herein.

REFERENCES

1. J. F. Briesmeister, editor, "MCNP – A General Monte Carlo Code for Neutron and Photon Transport Version 3A," Los Alamos National Laboratory manual LA–7396–M, Rev. 2 (September 1986).

2. S. P. Pederson, "Mean Estimation in Highly Skewed Samples," Los Alamos National Laboratory Report LA-12114-MS (1991).

3. R. A. Forster, "*A New Method of Assessing the Statistical Convergence of Monte Carlo Solutions,*" *Trans. Am. Nucl. Soc.*, **64**, 305 (1991).

4. Francis H. Clark, "The Exponential Transform as an Importance Sampling Device - A Review," Oak Ridge National Laboratory Report ORNL-RSIC-14 (Jan. 1966).

5. Iván Lux and László Koblinger, "*Monte Carlo Particle Transport Methods: Neutron and Photon Calculations,*" CRC Press, Inc. (1991).

6. Analytic Comparison of Monte Carlo Geometry Splitting and Exponential Transform, Thomas E. Booth, Trans. Am. Nuc. Soc., Vol. 64 p303, Nov. 10-14, 1991, San Francisco, CA.

7. Analytic Score Comparison of Geometry Splitting and Exponential Transform for a Simple Monte Carlo Problem, Thomas E. Booth, Los Alamos National Laboratory Report LA-12258 (1992).

8. Analytic Monte Carlo Score Distributions for Future Statistical Confidence Interval Studies, Thomas E. Booth, Nuclear Science and Engineering 112, p. 159-169 (1992).

9. "Elementary Differential Equations and Boundary Value Problems", Second Edition p. 288, William E. Boyce and Richard C. DiPrima John Wiley and Sons (1969)

APPENDIX A

The following FORTRAN program with $f = .25$, $b = .25$, and $q = .5$ computed the critical thicknesses (for finite second moment using Eq. 76) shown in Table I (see p. 46). Table I shows the critical thickness dependence on transform parameter p and scattering cross section σ_s. A negative entry for a particular transform parameter p and scattering cross section σ_s means that the critical thickness is infinite. That is, the second moment is finite for all thicknesses. The results are for analog capture.

```
      program series(tty,input=tty,output=tty,out,tape4=out)
      dimension tcrit(100,100)
c   computes critical thickness for finite variance and exponential transform
c   sig=total cross section
c   sigs=scattering cross section
c   p=exponential transform parameter
c   f=probability of forward scattering (no direction change)
c   b=probability of backward scattering
c   q=probability of 90 degree scattering
      write(*,*)'enter f,b,q=?'
      read(*,*)f,b,q
      sig=1
      do 800 i=1,9
      sigs=.1*i
      do 700 j=1,49
      p=.02*j
      za=(sigs/(1-p))*(f+ sigs*q**2/(2*sig) / (1-sigs*(f+b)/sig)  )
     1   -sig*(1+p)
      zb=(-sigs/(1-p))*( b+ sigs*q**2/(2*sig) / (1-sigs*(f+b)/sig) )
      zg=sig*(1-p)
     1   -(sigs/(1+p))*(f+ sigs*q**2/(2*sig) / (1-sigs*(f+b)/sig)  )
      ze=(sigs/(1+p))*( b+ sigs*q**2/(2*sig) / (1-sigs*(f+b)/sig) )
      zm=abs( (za-zg)**2+4*zb*ze )
      rz2=.5*( -(za+zg)+ri*sqrt(zm) )+zg
      zirt2=.5*sqrt(zm)
      zrrt2=.5*( -(za+zg) )+zg
      zth=atan(zirt2/zrrt2)
c     write(4,*)'za,zb,zg,ze=',za,zb,zg,ze
c     write(4,*)'zm,zirt2,zrrt2,zth=',zm,zirt2,zrrt2,zth
      zr1=.5*( -(za+zg) )
      zr2=.5*( -(za+zg) )
      d=(za-zg)**2+4*zb*ze
      if(d.lt.0)go to 561
      zr1=zr1-.5*sqrt(d)
      zr2=zr2+.5*sqrt(d)
      ztc=alog( (zr1+zg)/(zr2+zg) )/(zr2-zr1)
```

```
      write(4,*)'sigs,p,real ztc ',i,j,sigs,p,ztc
      tcrit(i,j)=ztc
      go to 700
  561 continue
c  complex roots
      if(zth.le.0)ztc=(-zth)/(.5*sqrt(zm))
      if(zth.gt.0)ztc=(3.141592653589793-zth)/(.5*sqrt(zm))
      write(4,*)'sigs,p,complex ztc ',i,j,sigs,p,ztc
      tcrit(i,j)=ztc
  700 continue
  800 continue
      write(4,2000)
 2000 format(1h1)
      do 900 j=1,49
      write(4,1000)(tcrit(i,j),i=1,9)
 1000 format(1p9e14.5)
  900 continue
      end
```

APPENDIX B

The following FORTRAN program with analog capture computed the first four score moments for the problem described in Table II (see p. 47). The theoretical moments come from Eq. 79 and the sample moments come from the program run with 10 million samples. Note that the higher moments are more difficult to estimate correctly, and thus the fourth moment is still not adequately estimated even with 10 million samples. (This program also provides Monte Carlo estimates of the actual score probability distribution F_{mn}.)

```
      program series(tty,input=tty,output=tty,outmc,tape4=outmc)
      common/teb/rm(100),theorym(100),fmn(0:100,0:100)
c  computes all tri-directional scattering analytic and empirical moments
c  sig=total cross section
c  sigs=scattering cross section
c  t=slab thickness
c  f=probability of forward scattering (no direction change)
c  b=probability of backward scattering
c  q=probability of 90 degree scattering
      write(*,*)'enter p temporarily='
      read(*,*)p
      write(*,*)'enter 0 for analog 1 for implicit capture'
      read(*,*)impl
      write(*,*)'enter sig,sigs,t=?'
      read(*,*)sig,sigs,t
      write(*,*)'enter sigforward='
      read(*,*)sigp
      write(*,*)'enter sigbackward='
      read(*,*)sigm
      write(*,*)'enter sigperpendicular='
      read(*,*)sig0
      write(*,*)'enter f,b,q=?'
      read(*,*)f,b,q
      write(*,*)'enter number of moments to compute=?'
      read(*,*)mom
      do 11 ir=1,mom
      g=sigs/sig
```

```
      v=1
      if(impl.eq.0)go to 543
      g=1
      v=sigs/sig
  543 continue
      dee=(g*v**ir*q**2)/(2*(1-g*v**ir*(f+b)))
      za=g*sig*v**ir*(1-p)**(-ir+1)*(f+dee)-sig*(1+(ir-1)*p)
      zb=-(1-p)**(-ir+1)*g*sig*v**ir*(b+dee)
      zg=sig*(1-(ir-1)*p)-(g*sig*v**ir*(1+p)**(-ir+1))*(f+dee)
      ze=(1+p)**(-ir+1)*g*sig*v**ir*(b+dee)
cccccccccccccccccc  new equations  cccccccccc
      gee=v**ir*g*sig0*(sig/sig0)**ir/(sig0+ir*(sig-sig0))
      dee=.5*q**2*gee/(1-gee*(f+b))
      write(*,*)'za=',za
      za=(sigp/sig)**(-ir+1)*sig*g*v**ir*(f+dee)-(sig*ir-sigp*(ir-1))
      write(*,*)'za=',za
      write(*,*)'zb=',zb
      zb=-(sigp/sig)**(-ir+1)*sig*g*v**ir*(b+dee)
      write(*,*)'zb=',zb
      write(*,*)'zg=',zg
      zg=sig*ir-sigm*(ir-1)-(sigm/sig)**(-ir+1)*sig*g*v**ir*(f+dee)
      write(*,*)'zg=',zg
      write(*,*)'ze=',ze
      ze=(sigm/sig)**(-ir+1)*sig*g*v**ir*(b+dee)
      write(*,*)'ze=',ze
ccccccccccccccccccc end new equations  cccccc
      zm=abs( (za-zg)**2+4*zb*ze )
      zirt2=.5*sqrt(zm)
      zrrt2=.5*( -(za+zg) )+zg
      zth=atan(zirt2/zrrt2)
c      write(4,*)'za,zb,zg,ze=',za,zb,zg,ze
c      write(4,*)'zm,zirt2,zrrt2,zth=',zm,zirt2,zrrt2,zth
      zr1=.5*( -(za+zg) )
      zr2=.5*( -(za+zg) )
      d=(za-zg)**2+4*zb*ze
      if(d.le.0)go to 561
```

```
c  real roots
      zr1=zr1-.5*sqrt(d)
      zr2=zr2+.5*sqrt(d)
      ztc=alog( abs((zr1+zg)/(zr2+zg)) )/(zr2-zr1)
      write(4,*)'sigs,sigp,sig0,sigm,real ztc '
     1 ,i,j,sigs,sigp,sig0,sigm,ztc
      rnum=-(zr1+zg)*exp(zr1*x)+(zr2+zg)*exp(zr2*x)
      rden=-(zr1+zg)*exp(zr1*t)+(zr2+zg)*exp(zr2*t)
      rn0=rnum/rden
      write(4,*)ir,'theoretical moment=',rn0
      theorym(ir)=rn0
      go to 700
  561 continue
c  complex roots
      if(zth.le.0)ztc=(-zth)/(.5*sqrt(zm))
      if(zth.gt.0)ztc=(3.141592653589793-zth)/(.5*sqrt(zm))
      write(4,*)'sigs,sigp,sig0,sigm,complex ztc '
      1 ,sigs,sigp,sig0,sigm,ztc
      y=.5*sqrt(zm)
      x=0
      rnum=exp(zr1*x)*( (zr1+zg)*sin(y*x)+y*cos(y*x) )
      rden=exp(zr1*t)*( (zr1+zg)*sin(y*t)+y*cos(y*t) )
      rn0=rnum/rden
      write(4,*)ir,'theoretical moment=',rn0
      theorym(ir)=rn0
  700 continue
   11 continue
      write(*,*)'enter number of particles (in thousands)=?'
      read(*,*)nppk
      npp=1000*nppk
      do 12 ir=1,mom
      rm(ir)=0.
   12 continue
      do 804 n1000=1,1000
      do 803 nps=1,nppk
      mu=1
```

```
      x=0
      m=0
      n=0
      w=1
  814 continue
c  distance to collision
      xo=x
      if(mu.eq.0)sigfict=sig0
      if(mu.eq.-1)sigfict=sigm
      if(mu.eq.1)sigfict=sigp
      s=-alog(ranf())/sigfict
      x=x+mu*s
      if(x.gt.t)go to 810
      if(x.lt.0)go to 803
      w=w*sig*exp(-sig*s)/(sigfict*exp(-sigfict*s))
c  reduce weight if implicit capture
      if(impl.eq.0)go to 877
      w=w*sigs/sig
      go to 876
  877 continue
c  check for absorption
      if(ranf().gt.sigs/sig)go to 803
  876 continue
      rn=ranf()
      if(mu.eq.0)go to 900
      if(mu.eq.1)go to 910
c  mu=-1
      n=n+1
      if(n.gt.100)stop 14
      if(rn.lt.f)go to 814
      mu=0
      if(rn.lt.f+q)go to 814
      mu=1
      go to 814
  900 continue
c  mu=0
```

```
      if(rn.lt.f+b)go to 814
c  scatter right or left with equal probability
      mu=-1
      if(ranf().gt.0.5)mu=1
      go to 814
  910 continue
c  mu=1
      m=m+1
      if(m.gt.100)stop 13
      if(rn.lt.f)go to 814
      mu=0
      if(rn.lt.f+q)go to 814
      mu=-1
       go to 814
   810 continue
c  penetrate the slab at x=t
      s=t-xo
      fmn(m,n)=fmn(m,n)+1
      w=w*exp(-sig*s)/exp(-sigfict*s)
      do 612 ir=1,mom
      rm(ir)=rm(ir)+w**ir
  612 continue
  803 continue
  804 continue
      do 712 ir=1,mom
      rm(ir)=rm(ir)/npp
      write(4,1000)ir,rm(ir),theorym(ir)
      write(*,1000)ir,rm(ir),theorym(ir)
 1000 format(i5,'-th moment=',1pe13.6,' theoretical moment=',e13.6)
  712 continue
      sd=sqrt((rm(2)-rm(1)**2)/npp)
      write(4,*)'mean, standard deviation=',rm(1),sd
      write(*,*)'mean, standard deviation=',rm(1),sd
      do 986 m=0,20
      do 985 n=0,20
      fmn(m,n)=fmn(m,n)/npp
```

```
  985 continue
  986 continue
      do 988 m=0,20
      write(4,3000)(m,(fmn(m,n),n=0,8))
 3000 format(i5,1p9e14.6)
  988 continue
      end
```

APPENDIX C

The following FORTRAN program with analog capture computed the theoretical score distribution for the problem indicated in Table III (see p. 48) using Eqs. 116, 117, 118, 127, 128, 129, and 106. ($F_{mn}(s)$ is evaluated at $s = T$.) The sample score probabilities come from the same 10 million sample run of the program referred to in Appendix B.

```
      program coef(tty,input=tty,output=tty,out,tape4=out)
      common/teb/a(-1:20,-1:20,-1:20),b(-1:20,-1:20,-1:20),
     1c(-1:20,-1:20,-1:20),d(-1:20,-1:20,-1:20),fact(0:30),f(0:20,0:20)
      fact(0)=1
      do 20 i=1,20
   20 fact(i)=i*fact(i-1)
      write(*,*)'enter 0 for analog 1 for implicit capture'
      read(*,*)impl
      write(*,*)'enter sig,sigs,p,t=?'
      read(*,*)sig,sigs,p,t
      write(*,*)'entor f,b,q=?'
      read(*,*)forw,back,r90
      g=sigs/sig
      v=1
      if(impl.eq.0)go to 543
      g=1
      v=sigs/sig
  543 continue
      q=(g*r90**2)/(1-(forw+back)*g)
      al=2*forw+q
      be=2*back+q
      sigp=sig*(1-p)
      sigm=sig*(1+p)
      rk=g*sigp/2.
      rm=g*sigm/2
      write(*,*)'rk,rm,rk*rm=',rk,rm,rk*rm
      do 100 m=0,20
      do 100 n=0,20
      do 100 j=0,20
```

```
      a(m,n,j)=1.7e123
      b(m,n,j)=1.7e123
      c(m,n,j)=1.7e123
      d(m,n,j)=1.7e123
  100 continue
      do 22 i=0,20
      do 21 j=0,20
      a(0,i,j)=0
      b(0,i,j)=0
      c(i,0,j)=0
      d(i,0,j)=0
      b(i,0,j)=0
   21 continue
   22 continue
      do 72 m=0,20
      do 62 j=0,m
      a(m,0,j)=0
   62 continue
      a(m,0,m)=rk**m*al**m/fact(m)
   72 continue
c     a(1,0,1)=rk
c     d(0,1,0)=(-rm/(2*sig))*exp(-2*sig*t)
c     a(1,1,0)=( (rk*rm)/(2*sig)**2 )*exp(-2*sig*t)
c     c(0,1,0)=rm/(2*sig)
c     a(1,1,1)=(rk*rm)/(2*sig)
c     b(1,1,0)=-( (rk*rm)/(2*sig)**2 )*exp(-2*sig*t)
c     c(1,1,0)=(rk*rm)/(2*sig)**2
c     c(1,1,1)=(rk*rm)/(2*sig)
c     d(1,1,0)=-( (rk*rm)/(2*sig)**2 )*exp(-2*sig*t)*(1+2*sig*t)
c     a(2,1,0)=((2*rk*rk*m)/(2*sig)**3)*exp(-2*sig*t)*(1+sig*t)
c     a(2,1,1)=((rk*rk*m)/(2*sig)**2)*(1+exp(-2*sig*t))
c     b(2,1,0)=-((2*rk*rk*m)/(2*sig)**3)*exp(-2*sig*t)*(1+sig*t)
c     a(2,0,2)=rk**2/2
      do 900 ir=1,10000000
      m=21*ranf()
      n=21*ranf()
```

```
      j3=21*ranf()
c  choose formula to try to apply at random
      irform=1+ranf()*6
      go to(111,112,113,114,115,116)irform
 111 continue
c  try to compute a(m,n,0)
      m=max(1,m)
      n=max(1,n)
      if(abs(a(m,n,0)).lt.1.e50)go to 900
      sum=0
      do 300 j=0,n-1
      if(abs(b(m-1,n,j)).gt.1.e50)go to 900
      if(abs(d(m-1,n,j)).gt.1.e50)go to 900
      sum=sum+(al*b(m-1,n,j)+be*d(m-1,n,j))*(-1)**(j+1)
     1 *(2*sig)**(-(j+1))*fact(j)
 300 continue
      if(abs(sum).gt.1.e50)go to 900
      a(m,n,0)=rk*sum
c       write(*,*)'m,n,a(m,n,0)=',m,n,a(m,n,0)
      go to 900
 112 continue
c  try to compute a(m,n,j)
      j=max(1,j3)
      j=min(j,m)
      if(abs(a(m,n,j)).lt.1.e50)go to 900
      do 410 j=1,m
      if(abs(a(m-1,n,j-1)).gt.1.e50)go to 900
      if(abs(c(m-1,n,j-1)).gt.1.e50)go to 900
      a(m,n,j)=(rk/j)*(al*a(m-1,n,j-1)+be*c(m-1,n,j-1))
c       write(*,*)'m,n,j,a(m,n,j)=',m,n,j,a(m,n,j)
 410 continue
      go to 900
 113 continue
c  try to compute  b(m,n,j3)
      n=max(1,n)
      m=max(1,m)
```

```
      j3=min(j3,n-1)
      if(abs(b(m,n,j3)).lt.1.e50)go to 900
      k=j3
      sum=0
      do 430 j=k,n-1
      if(abs(b(m-1,n,j)).gt.1.e50)go to 900
      if(abs(d(m-1,n,j)).gt.1.e50)go to 900
      sum=sum+(al*b(m-1,n,j)+be*d(m-1,n,j))*(2*sig)**(k-j-1)*(-1)**(j+k)
     1 *fact(j)/fact(k)
  430 continue
      b(m,n,k)=rk*sum
c      write(*,*)'m,n,k,b(m,n,k)=',m,n,k,b(m,n,k)
      go to 900
  114 continue
c  try to compute  c(m,n,j3)
      j3=min(j3,m)
      n=max(1,n)
      k=j3
      if(abs(c(m,n,j3)).lt.1.e50)go to 900
      sum=0
      do 460 j=k,m
      if(abs(c(m,n,k)).lt.1.e50)go to 900
      if(abs(a(m,n-1,j)).gt.1.e50)go to 900
      if(abs(c(m,n-1,j)).gt.1.e50)go to 900
      sum=sum+(be*a(m,n-1,j)+al*c(m,n-1,j))*(2*sig)**(k-j-1)
     1   *fact(j)/fact(k)
  460 continue
      c(m,n,k)=rm*sum
c      write(*,*)'m,n,k,c(m,n,k)=',m,n,k,c(m,n,k)
      go to 900
  115 continue
c  try to compute  d(m,n,0)
      n=max(n,1)
      sum1=0
      if(abs(d(m,n,0)).lt.1.e50)go to 900
      if(n.eq.1)go to 514
```

```
      do 510 j=0,n-2
      if(abs(b(m,n-1,j)).gt.1.e50)go to 900
      if(abs(d(m,n-1,j)).gt.1.e50)go to 900
      sum1=sum1+(be*b(m,n-1,j)+al*d(m,n-1,j))*t**(j+1)/(j+1)
  510 continue
  514 continue
      sum2=0
      do 540 k=0,m
      do 530 j=k,m
      if(abs(a(m,n-1,j)).gt.1.e50)go to 900
      if(abs(c(m,n-1,j)).gt.1.e50)go to 900
      sum2=sum2+(be*a(m,n-1,j)+al*c(m,n-1,j))*(2*sig)**(k-j-1)
     1   *(fact(j)/fact(k))*t**k
  530 continue
 540 continue
      d(m,n,0)=rm*sum1-rm*exp(-2*sig*t)*sum2
c      write(*,*)'m,n,d(m,n,0)=',m,n,d(m,n,0)
      go to 900
  116 continue
c  try to compute  d(m,n,i)
      i=j3
      n=max(1,n)
      i=min(i,n-1)
      i=max(i,1)
      if(i.ge.n)go to 900
      if(abs(d(m,n,i)).lt.1.e50)go to 900
      if(abs(b(m,n-1,i-1)).gt.1.e50)go to 900
      if(abs(d(m,n-1,i-1)).gt.1.e50)go to 900
      d(m,n,i)=-(rm/i)*(be*b(m,n-1,i-1)+al*d(m,n-1,i-1))
c      write(*,*)'ir=',ir
c      write(*,*)'m,n,i,d(m,n,i)=',m,n,i,d(m,n,i)
  900 continue
      a210=2*(rk*rk*rm/(2*sig)**3)*exp(-2*sig*t)*(1+sig*t)
c      write(*,*)'b(1,1,0),d(1,1,0)=',b(1,1,0),d(1,1,0)
c      write(*,*)'a210,a(2,1,0)=',a210,a(2,1,0)
      a211=(rk*rk*rm/(2*sig)**2)*(1+exp(-2*sig*t))
```

```
c      write(*,*)'a211,a(2,1,1)=',a211,a(2,1,1)
      a212=(rk*rk*rm/(2*sig))
c      write(*,*)'a212,a(2,1,2)=',a212,a(2,1,2)
      b210=-(2*rk*rk*rm/(2*sig)**3)*exp(-2*sig*t)*(1+sig*t)
c      write(*,*)'b210,b(2,1,0)=',b210,b(2,1,0)
      write(4,2000)
 2000 format('  m  n  j',
     1'    a(m,n,j)      b(m,n,j)      c(m,n,j)      d(m,n,j)')
      do 930 m=0,7
      do 920 n=0,7
      do 910 j=0,7
c     if(abs(a(m,n,j)).gt.1.e50)a(m,n,j)=0
c     if(abs(b(m,n,j)).gt.1.e50)b(m,n,j)=0
c     if(abs(c(m,n,j)).gt.1.e50)c(m,n,j)=0
c     if(abs(d(m,n,j)).gt.1.e50)d(m,n,j)=0
      if(a(m,n,j).eq.0 .and.  b(m,n,j).eq.0
     1   .and.  c(m,n,j).eq.0  .and.  d(m,n,j).eq.0)go to 910
      const=1
      a(m,n,j)=a(m,n,j)*const
      b(m,n,j)=b(m,n,j)*const
      c(m,n,j)=c(m,n,j)*const
      d(m,n,j)=d(m,n,j)*const
      write(4,1000)m,n,j,a(m,n,j),b(m,n,j),c(m,n,j),d(m,n,j)
  910 continue
  920 continue
  930 continue
 1000 format(3i3,1p5e14.6)
      do 970 m=0,20
      do 960 n=0,20
      sump=0
      summ=0
      do 940 j=0,m
      sump=sump+a(m,n,j)*t**j
  940 continue
      if(n.eq.0)go to 952
      do 950 j=0,n-1
```

```
      summ=summ+b(m,n,j)*t**j
  950 continue
  952 continue
      f(m,n)=exp(-sigp*t)*sump+exp(sigm*t)*summ
c     f(m,n)=fact(m)*fact(n)*f(m,n)/(rk**m*rm**n)
  960 continue
  970 continue
      do 980 m=0,20
      do 975 n=0,20
      smn=(1-p)**(-m)*(1+p)**(-n)*exp(-p*sig*t)
      write(4,3000)m,n,smn,f(m,n)
 3000 format(2i5,1p7e14.6)
  975 continue
  980 continue
      do 981 m=0,5
      write(*,3001)m,(f(m,n),n=0,5)
 3001 format(i5,1p7e14.6)
  981 continue
      end
```

TABLE I

CRITICAL THICKNESS FOR FINITE VARIANCES AS A FUNCTION OF SCATTERING PROBABILITY AND EXPONENTIAL TRANSFORM PARAMETER

				Scattering Probability					
σ_s=.1	σ_s=.2	σ_s=.3	σ_s=.4	σ_s=.5	σ_s=.6	σ_s=.7	σ_s=.8	σ_s=.9	exponential transform parameter
-4.42165E+00	-3.73870E+00	-3.33456E+00	-3.04127E+00	-2.80755E+00	-2.61035E+00	-2.43732E+00	-2.28100E+00	-2.13642E+00	
-4.42115E+00	-3.73876E+00	-3.33417E+00	-3.04094E+00	-2.80727E+00	-2.61012E+00	-2.43715E+00	-2.28088E+00	-2.13636E+00	
-4.42030E+00	-3.73803E+00	-3.33353E+00	-3.04039E+00	-2.80681E+00	-2.60974E+00	-2.43688E+00	-2.28068E+00	-2.13626E+00	
-4.41912E+00	-3.73700E+00	-3.33263E+00	-3.03962E+00	-2.80616E+00	-2.60922E+00	-2.43648E+00	-2.28041E+00	-2.13612E+00	
-4.41760E+00	-3.73567E+00	-3.33148E+00	-3.03863E+00	-2.80533E+00	-2.60854E+00	-2.43594E+00	-2.28006E+00	-2.13595E+00	p=.1
-4.41573E+00	-3.73406E+00	-3.33007E+00	-3.03742E+00	-2.80431E+00	-2.60772E+00	-2.43532E+00	-2.27964E+00	-2.13574E+00	
-4.41361E+00	-3.73212E+00	-3.32838E+00	-3.03598E+00	-2.80311E+00	-2.60675E+00	-2.43450E+00	-2.27916E+00	-2.13551E+00	
-4.41094E+00	-3.72988E+00	-3.32646E+00	-3.03433E+00	-2.80172E+00	-2.60563E+00	-2.43374E+00	-2.27860E+00	-2.13526E+00	
-4.40801E+00	-3.72734E+00	-3.32425E+00	-3.03244E+00	-2.80015E+00	-2.60437E+00	-2.43280E+00	-2.27798E+00	-2.13500E+00	
-4.40471E+00	-3.72449E+00	-3.32178E+00	-3.03034E+00	-2.79840E+00	-2.60297E+00	-2.43178E+00	-2.27732E+00	-2.13473E+00	p=.2
-4.40106E+00	-3.72131E+00	-3.31904E+00	-3.02800E+00	-2.79646E+00	-2.60143E+00	-2.43068E+00	-2.27661E+00	-2.13447E+00	
-4.39700E+00	-3.71781E+00	-3.31603E+00	-3.02544E+00	-2.79434E+00	-2.59976E+00	-2.42941E+00	-2.27587E+00	-2.13423E+00	
-4.39256E+00	-3.71398E+00	-3.31274E+00	-3.02265E+00	-2.79204E+00	-2.59796E+00	-2.42811E+00	-2.27509E+00	-2.13401E+00	
-4.38773E+00	-3.70982E+00	-3.30916E+00	-3.01963E+00	-2.78957E+00	-2.59603E+00	-2.42674E+00	-2.27431E+00	-2.13384E+00	
-4.38248E+00	-3.70532E+00	-3.30530E+00	-3.01638E+00	-2.78692E+00	-2.59398E+00	-2.42530E+00	-2.27352E+00	-2.13374E+00	p=.3
-4.37682E+00	-3.70046E+00	-3.30116E+00	-3.01291E+00	-2.78410E+00	-2.59182E+00	-2.42382E+00	-2.27274E+00	-2.13373E+00	
-4.37071E+00	-3.69526E+00	-3.29671E+00	-3.00920E+00	-2.78111E+00	-2.58955E+00	-2.42230E+00	-2.27201E+00	-2.13383E+00	
-4.36416E+00	-3.68965E+00	-3.29197E+00	-3.00527E+00	-2.77796E+00	-2.58720E+00	-2.42070E+00	-2.27132E+00	-2.13407E+00	
-4.35713E+00	-3.68367E+00	-3.28693E+00	-3.00110E+00	-2.77466E+00	-2.58478E+00	-2.41922E+00	-2.27074E+00	-2.13450E+00	
-4.34963E+00	-3.67731E+00	-3.28156E+00	-2.99671E+00	-2.77121E+00	-2.58230E+00	-2.41771E+00	-2.27027E+00	-2.13516E+00	p=.4
-4.34161E+00	-3.67055E+00	-3.27592E+00	-2.99208E+00	-2.76762E+00	-2.57972E+00	-2.41626E+00	-2.26996E+00	-2.13607E+00	
-4.33307E+00	-3.66338E+00	-3.26994E+00	-2.98720E+00	-2.76391E+00	-2.57716E+00	-2.41488E+00	-2.26984E+00	-2.13734E+00	
-4.32397E+00	-3.65578E+00	-3.26364E+00	-2.98221E+00	-2.76010E+00	-2.57460E+00	-2.41364E+00	-2.27000E+00	-2.13902E+00	
-4.31429E+00	-3.64770E+00	-3.25703E+00	-2.97698E+00	-2.75621E+00	-2.57206E+00	-2.41257E+00	-2.27048E+00	-2.14120E+00	
-4.30400E+00	-3.63916E+00	-3.25008E+00	-2.97152E+00	-2.75226E+00	-2.56967E+00	-2.41175E+00	-2.27130E+00	2.22916E+01	p=.5
-4.29307E+00	-3.63019E+00	-3.24282E+00	-2.96601E+00	-2.74828E+00	-2.56736E+00	-2.41125E+00	-2.27280E+00	1.43186E+01	
-4.28146E+00	-3.62071E+00	-3.23524E+00	-2.96015E+00	-2.74436E+00	-2.56532E+00	-2.41110E+00	-2.27467E+00	1.08237E+01	
-4.26913E+00	-3.61072E+00	-3.22736E+00	-2.95426E+00	-2.74046E+00	-2.56354E+00	-2.41160E+00	-2.27774E+00	8.90844E+00	
-4.25604E+00	-3.60022E+00	-3.21916E+00	-2.94830E+00	-2.73677E+00	-2.56216E+00	-2.41272E+00	-2.28182E+00	7.52468E+00	
-4.24213E+00	-3.58917E+00	-3.21068E+00	-2.94232E+00	-2.73330E+00	-2.56132E+00	-2.41473E+00	-2.28677E+00	6.48686E+00	p=.6
-4.22736E+00	-3.57756E+00	-3.20198E+00	-2.93638E+00	-2.73016E+00	-2.56120E+00	-2.41784E+00	-2.29351E+00	5.68528E+00	
-4.21165E+00	-3.56542E+00	-3.19302E+00	-2.93058E+00	-2.72781E+00	-2.56202E+00	-2.42240E+00	-2.30220E+00	5.02533E+00	
-4.19496E+00	-3.55271E+00	-3.18384E+00	-2.92506E+00	-2.72570E+00	-2.56410E+00	-2.42863E+00	1.60536E+01	4.47034E+00	
-4.17717E+00	-3.53945E+00	-3.17476E+00	-2.91988E+00	-2.72492E+00	-2.56785E+00	-2.43770E+00	1.02570E+01	3.99402E+00	
-4.15825E+00	-3.52564E+00	-3.16572E+00	-2.91563E+00	-2.72560E+00	-2.57362E+00	-2.44981E+00	7.69426E+00	3.57798E+00	p=.7
-4.13808E+00	-3.51130E+00	-3.15680E+00	-2.91231E+00	-2.72801E+00	-2.58200E+00	-2.46628E+00	6.14750E+00	3.20822E+00	
-4.11654E+00	-3.49671E+00	-3.14882E+00	-2.91053E+00	-2.73324E+00	-2.59603E+00	-2.48872E+00	5.07392E+00	2.87837E+00	
-4.09396E+00	-3.48179E+00	-3.14128E+00	-2.91102E+00	-2.74230E+00	-2.61485E+00	1.31063E+01	4.28886E+00	2.57832E+00	
-4.06922E+00	-3.46688E+00	-3.13551E+00	-2.91488E+00	-2.75688E+00	-2.64213E+00	8.08088E+00	3.63467E+00	2.30381E+00	
-4.04319E+00	-3.45240E+00	-3.13230E+00	-2.92378E+00	-2.77987E+00	-2.68183E+00	5.83943E+00	3.08679E+00	2.04893E+00	p=.8
-4.01557E+00	-3.43908E+00	-3.13322E+00	-2.94041E+00	-2.81503E+00	1.91878E+01	4.50082E+00	2.64679E+00	1.81377E+00	
-3.98647E+00	-3.42813E+00	-3.14088E+00	-2.96867E+00	-2.87071E+00	8.14608E+00	3.56798E+00	2.25882E+00	1.59221E+00	
-3.95628E+00	-3.42192E+00	-3.16042E+00	-3.01984E+00	-2.96163E+00	5.26879E+00	2.88128E+00	1.91088E+00	1.38274E+00	
-3.92801E+00	-3.42493E+00	-3.20105E+00	-3.10892E+00	1.02880E+01	3.75190E+00	2.29401E+00	1.58919E+00	1.18308E+00	
-3.89823E+00	-3.44679E+00	-3.28363E+00	-3.27882E+00	5.24100E+00	2.75406E+00	1.82083E+00	1.31358E+00	9.91066E-01	p=.9
-3.87873E+00	-3.51128E+00	-3.46451E+00	8.47330E+00	3.29856E+00	2.01930E+00	1.41088E+00	1.04756E+00	8.04416E-01	
-3.80134E+00	-3.68281E+00	3.06519E+01	3.81142E+00	2.13008E+00	1.43369E+00	1.04468E+00	7.95080E-01	6.20422E-01	
-4.01987E+00	-4.37580E+00	4.01744E+00	2.02128E+00	1.31000E+00	9.37461E-01	7.08776E-01	5.48482E-01	4.36271E-01	
-5.13388E+00	3.13167E+00	1.46477E+00	9.23253E-01	6.81700E-01	4.88112E-01	3.78594E-01	3.00051E-01	2.41003E-01	

TABLE II

COMPARISON OF THE FIRST FOUR SAMPLE MOMENTS VERSUS THE THEORETICAL MOMENTS

sample 1-st moment= 1.671871E-02 theoretical moment= 1.669347E-02

sample 2-nd moment= 3.260687E-03 theoretical moment= 3.252548E-03

sample 3-rd moment= 1.446749E-03 theoretical moment= 1.506766E-03

sample 4-th moment= 1.942878E-03 theoretical moment= 4.377704E-03

Problem: σ=1 σ=.5 σ_+=.5 σ_0=1.0 σ_-=1.5 T = 5.0

10 Million Samples

Isotropic Scattering: f=.25, b=.25, q= = .5

TABLE III

COMPARISON OF THEORETICAL VERSUS SAMPLE SCORE PROBABILITIES (F_{mn})

Theoretical Score Probabilities F_{mn}

	n=0	n=1	n=2	n=3	n=4	n=5
0	8.208500E-02	0.000000E+00	0.000000E+00	0.000000E+00	0.000000E+00	0.000000E+00
1	3.420208E-02	3.847754E-03	4.275551E-04	4.678280E-05	5.021469E-06	5.263604E-07
2	7.125434E-03	1.745749E-03	3.162212E-04	5.012644E-05	7.321306E-06	1.008919E-06
3	9.896436E-04	3.985871E-04	1.048559E-04	2.253313E-05	4.271736E-06	7.405441E-07
4	1.030879E-04	6.111302E-05	2.197593E-05	6.153942E-06	1.470503E-06	3.136504E-07
5	8.590656E-06	7.085730E-06	3.359252E-06	1.194472E-06	3.525779E-07	9.097949E-08

Sample Score Probabilities (10 million samples)

	n=0	n=1	n=2	n=3	n=4	n=5
0	8.232220E-02	0.000000E+00	0.000000E+00	0.000000E+00	0.000000E+00	0.000000E+00
1	3.423430E-02	3.832400E-03	4.392000E-04	4.320000E-05	4.000000E-06	6.000000E-07
2	7.111200E-03	1.729300E-03	3.177000E-04	4.980000E-05	6.800000E-06	1.300000E-06
3	1.005300E-03	3.902000E-04	1.067000E-04	2.450000E-05	4.900000E-06	1.000000E-06
4	1.027000E-04	6.020000E-05	2.230000E-05	7.300000E-06	1.500000E-06	3.000000E-07
5	9.800000E-06	6.100000E-06	4.100000E-06	1.100000E-06	5.000000E-07	0.000000E+00

Problem: Analog Capture σ=1 σ_s=.5 σ_+=.5 σ_0=1.0 σ_-=1.5 T=5.0