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Geometrical Splitting in Monte Carlo

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Through a direct statistical approach, analytic expressions are derived for the second moment, the variance ratio, and benefit functions of a model for n-surface geometric splitting. The model is general in that it can be applied to many geometric and material conditions, energy dependence, and biasing methods besides splitting. The model applies to any detector, provided that the detector region is separated from the source region. The model has the following limitations: (a) every source particle reaching the detector must cross all splitting surfaces, (b) particles are allowed to split only once on each surface, (c) weight-dependent biasing schemes are not included, and (d) reactions that bifurcate the particle are excluded.

The derived expressions depend linearly on n unknown constants that are bulk properties of the medium in a given problem. These constants may be estimated approximately from one small sample run invoking the point-surface approximation or from (n + 1) consecutive small sample runs.

Numerical examples are given in verification of the theory, and the possibility of using the expressions in an in-code optimization or self-optimizing code is discussed.

I. INTRODUCTION

In recent years the Monte Carlo method has matured and has been used extensively in particle transport problems. Many variance-reducing techniques, biasing methods, and estimators have been derived for general and specific applications. Powerful multipurpose codes now combine flexible geometry with elaborate cross-section libraries and can handle any reasonable three-dimensional transport problem. With the increasing speed and capability of modern computers, the Monte Carlo method, once recommended for use only "when no other method is available,"[1] has become a common tool for experts in the nucleonics field, as well as for general researchers using the method for a wide variety of design and analysis purposes.

It is appropriate now to consider the goals of Monte Carlo methodology. It appears to be a general consensus that development of new general variance-reducing methods will produce only marginal benefit. Efficient application of the powerful methods already implemented in multipurpose codes is the most pressing problem in the use of Monte Carlo. All variance-reduction methods contain external parameters that must be specified before calculation. Correct determination of these parameters is, in most cases, crucial to the efficiency of the calculation, and correct setting can improve efficiency by orders

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[1] M. CLARK, Jr. and K. F. HANSEN, *Numerical Methods of Reactor Analysis*, p. 241, Academic Press, Inc., New York (1964).

of magnitude, in some cases determining feasibility of a calculation. Misuse of these parameters, on the other hand, might cause not only inefficient calculation, but also biased and therefore incorrect results.

Let us define the problem in more specific terms. Let D denote the target response, the quantity to be estimated in the calculation. Let $(\bar{P}_1, \ldots, \bar{P}_k)$ denote a random walk of a particle, with $\bar{P}_i$ being a phase-space collision point and $\bar{P}_k$ the termination point of the particle's history. A probability density function (pdf) is attached to every track, describing the probability density for the occurrence of that track. In the analog case, the pdf is constructed from the analog transport kernels and is denoted by $\mu_a(P_1, \ldots, \bar{P}_k)$. In any biased scheme, one uses a "distorted" pdf to bring the particles more efficiently from the source to the detector. This new pdf includes one or more external parameters $(\alpha_1, \ldots, \alpha_n)$ and is denoted by $\mu(\bar{P}_1, \ldots, \bar{P}_k; \alpha_1, \ldots, \alpha_n)$. To each random walk, a score $w(\bar{P}_1, \ldots, \bar{P}_k; \alpha_1, \ldots, \alpha_n)$ is attached. This score is a random variable and is an unbiased estimator of the target response if, when averaged over all possible random walks with the biased pdf, it yields D. Thus,

$$D = \sum_{k=0}^{\infty} \int \ldots \int w(\bar{P}_1, \ldots, \bar{P}_k; \alpha_1, \ldots, \alpha_n) \times \mu(\bar{P}_1, \ldots, \bar{P}_k; \alpha_1, \ldots, \alpha_n) d\bar{P}_1 \ldots d\bar{P}_k \quad . \quad (1)$$

In a Monte Carlo calculation, random walks are sampled from the biased (or analog) pdf and the numerical average of the score serves as an estimate of D. The variance of the calculation is determined by the second moment of w or

$$S^2(\alpha_1, \ldots, \alpha_n) = \sum_{k=0}^{\infty} \int \ldots \int w^2(\bar{P}_1, \ldots, \bar{P}_k; \alpha_1, \ldots, \alpha_n) \times \mu(\bar{P}_1, \ldots, \bar{P}_k; \alpha_1, \ldots, \alpha_n) d\bar{P}_1 \ldots d\bar{P}_k \quad . \quad (2)$$

The first-moment D does not depend on the external parameters, but the second moment does. If w has a finite variance V_w, then the variance of the estimate of D, for instance, $\tilde{D}$, behaves as $V_D = V_w/N$, where N is the number of histories used in the calculation. Further, if $\tau(\alpha_1, \ldots, \alpha_n)$ is the average computer time required to process a single history, the total calculation time is $T(\alpha_1, \ldots, \alpha_n) = N \cdot \tau(\alpha_1, \ldots, \alpha_n)$. Thus, an adequate measure of the efficiency of the calculation can be defined as

$$q(\alpha_1, \ldots, \alpha_n) = V_D T = V_w \tau = [S^2(\alpha_1, \ldots, \alpha_n) - D^2] \cdot \tau(\alpha_1, \ldots, \alpha_n) \quad . \quad (3)$$

When biasing is required, the second moment per history is usually much larger than the square of the first moment; if not, biasing is not needed and analog Monte Carlo will suffice. Therefore, in Eq. (3), D^2 can be safely omitted and $q(\alpha_1, \ldots, \alpha_n)$ can be written as

$$q(\alpha_1, \ldots \alpha_n) = S^2(\alpha_1, \ldots, \alpha_n)\tau(\alpha_1, \ldots, \alpha_n) \quad . \quad (4)$$

The q is also referred to as the quality factor of the calculation, and $(S^2/N)^{1/2}100/D$ will be the percentage relative standard deviation (PRSD) of D. The term $(S^2/N)100^2/D^2 \times T$ can be interpreted as the computational time required to achieve a PRSD of 1% and, for a given problem, is proportional to q. Now the problem can be stated simply as that of finding the set of external parameters $(\alpha_1, \ldots, \alpha_n)$ that will minimize $q(\alpha_1, \ldots, \alpha_n)$.

Optimizing variance-reduction methods is an important goal of Monte Carlo methodology. At present, the use of biasing methods depends on user experience and can be compared to "flying an experimental aircraft with unknown flight characteristics."[2]

This problem might be approached by the most straightforward scanning method. Because both S^2 and τ can be estimated, as well as D, during the calculation, the total number of histories can be divided into small batches that systematically scan different sets of external parameters and converge to the optimum. However, this approach must be rejected because estimating S^2 by small batches is frequently unreliable and misleading. In most cases, the time required to obtain a reliable estimate of S^2 is sufficient also to obtain a satisfactory estimate of D. However, the concept of in-code optimization, that is, an optimization done during and within the Monte Carlo calculation of D, is very tempting. It would require a "built in" algorithm enabling the code to converge to an optimum, or near optimum, set of external parameters. An algorithm based solely on statistical information acquired during the calculation probably will not suffice; some external analytical knowledge must be added to attenuate the statistical fluctuations of S^2.

Another possible approach was explored in the development of an integral-transport-like equation for the second moment in analog Monte Carlo.[3] This excellent work stimulated further extensions of the equation to include biased Monte Carlo schemes, time-dependent problems, and a variety

[2]D. J. DUDZIAK, "An Assessment of Nucleonic Methods and Data for Fusion Reactors," *Proc. Topl. Mtg. Technology of Controlled Nuclear Fusion*, Richland, Washington, September 21-23, 1976, CONF-760935, U.S. Department of Energy (1977).

[3]H. J. AMSTER and M. J. DJOMEHRI, *Nucl. Sci. Eng.*, **60**, 131 (1976).

of estimators.[4-9] Analysis of the equations prompted conclusions regarding the relations between second moments of such estimators as the track-length estimator, expected leakage estimator, and collision estimator, with and without survival biasing. Exponential biasing was analyzed and, in fact, quality factor curves were derived for a monokinetic infinite-medium problem including fission and time dependence.[7] The value of this approach is undoubted. References show that, without solving the equation, one may derive by comparison relations between second moments of different methods. ("Relations" refers here to larger or smaller, but without indicating exact differences or ratios.)

Considerable insight into various biasing methods may be gained by investigating the second-moment equation; newly suggested biasing schemes may be tested for their quality factor by using simple benchmark problems for which solutions of the second-moment equation are easily derived. It is doubtful, however, that this approach can lead to in-code optimization because, for optimization, a detailed solution of the second-moment equation is required. The resulting equation is more complicated than the transport equation and any attempt to solve it by Monte Carlo and within Monte Carlo runs will probably require the crude straightforward scanning method discussed earlier. It might be possible to apply methods other than Monte Carlo, such as S_N, P_N, or other deterministic methods,[10] which require some linkage between Monte Carlo and the deterministic method because the target response D appears as a parameter in the second-moment equation. Most deterministic codes are limited to one- or two-dimensional geometries, so in many practical cases, the three-dimensional problem must somehow be reduced into a two- or one-dimensional approximation, introducing an additional user-dependent element—even then it is not clear that the combined two-dimensional and Monte Carlo calculations will provide the solution. (However, this possibility should be investigated.) In summary, the prospects of the second-moment equation appear to be limited in the context of in-code optimization, for which information obtained during the calculation is used iteratively to improve quality without extra time investment.

Another possibility is an attempt to obtain an approximate or exact expression for the second moment directly from the basic statistical considerations applied to a general statistical model of the biasing method in question. Through such an analysis, one may derive the functional relation between the second moment (and the time) and the external parameters. Such a relation will eventually involve problem-dependent constants that can be described as "bulk properties," or integral properties of the specific problem, and are easier to calculate than the target response D. If this is achieved, one can construct an algorithm in which the bulk properties are learned within the calculation and, together with the known functional dependence of the quality factor on the external parameters, serve in a self-improving algorithm.

Reference 11 gives an example of this approach, where an approximate simple analytic expression was derived for the second moment of the one-parameter exponential biasing case. The bulk parameters were the average number of collisions of a particle and the total number of particles reaching the detector within the important range of the Neumann spectrum. A self-optimizing algorithm for a direction-dependent exponential biasing was devised[12] and implemented in the general purpose MCNP code.[13] Although we have little experience in using the algorithm, when it was tested on a shielding problem of leakage through a 0.7-m-thick concrete wall with bent liquid sodium pipe, a near-optimum parameter was obtained with $<10\%$ of the sample required for the entire calculation.

In the following, we apply the direct statistical approach to a model of surface splitting, deriving an exact functional relation of the second moment (and the quality factor) to the splitting parameters of any number of splitting surfaces.

Surface splitting is one of the most commonly used variance-reduction techniques. It consists of one or more splitting surfaces situated between the source and the detector. Upon crossing a surface, the particle is split into ν secondary particles, each of which weighs $1/\nu$ of the total original weight. This method is usually combined with Russian Roulette[14] and may be used with other biasing

[4]T. E. BOOTH and H. J. AMSTER, *Nucl. Sci. Eng.*, **65**, 273 (1978).

[5]I. LUX, "Variances and Efficiency in Transport Monte Carlo," KFDI 1979-35, Hungarian Academy of Sciences, Budapest (1979).

[6]I. LUX, *Atomkernenergie*, **31**, 154 (1978).

[7]T. E. BOOTH and EDMOND D. CASHWELL, *Nucl. Sci. Eng.*, **71**, 128 (1979).

[8]I. LUX, *Nucl. Sci. Eng.*, **67**, 317 (1978).

[9]P. K. SARKAR and M. A. PRASAD, *Nucl. Sci. Eng.*, **70**, 243 (1979).

[10]RAYMOND JOHN JUZAITIS, "Minimizing the Cost of Splitting in Monte Carlo Radiation Transport Simulation," LA-8546-T, Los Alamos National Laboratory (1980).

[11]A. DUBI and D. J. DUDZIAK, *Nucl. Sci. Eng.*, **70**, 243 (1979).

[12]A. DUBI and D. J. DUDZIAK, Los Alamos National Laboratory, unpublished data (1978).

[13]"MCNP—A General Monte Carlo Code for Neutron and Photon Transport," LA-7396-M, Los Alamos National Laboratory (July 1978).

[14]A. DUBI, *Nucl. Sci. Eng.*, **72**, 108 (1979).

methods. Reference 15 describes the analysis of a simple one-dimensional, one-surface monoenergetic problem in which each collision results in absorption; thus, the leakage consists of only uncollided particles.[16]

Section II is an analysis of the one-surface case. In Sec. III, we analyze the two-surface case and extend it to the n-surface model. Some numerical examples are cited to verify the theory, and possible ways of using the theory to obtain an in-code optimization algorithm are discussed.

II. ONE-SURFACE SPLITTING

A source region Q is separated from a detector region D and one splitting surface is in the medium between them (Fig. 1). Where splitting is not applied, we define these quantities: P_{qd} is the probability of a source particle reaching the detector region; w is the contribution of a particle that reached the detector (w includes both any accumulated weight due to biasing and the contribution to D in the detector using any estimator of D); $f(w)$ is the pdf of w. We then write the first moment as

$$D = P_{qd} \int_0^\infty f(w) w dw \ , \tag{5}$$

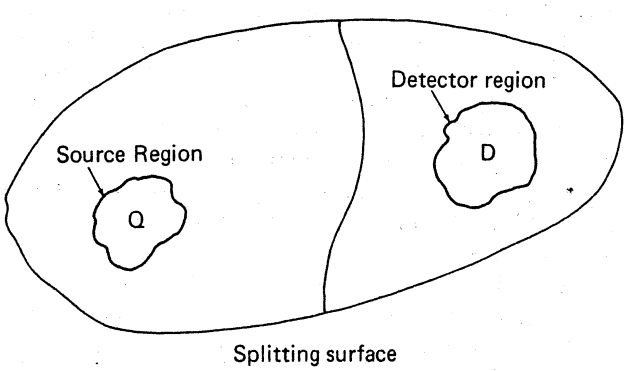


Fig. 1. General geometry.

assuming no negative contribution. Note that $f(w)$ is a conditional pdf only of those particles that reached the detector region.

The second moment is then given by

$$S_1^2 = P_{qd} \int_0^\infty w^2 f(w) dw \ . \tag{6}$$

To introduce splitting on the surface, we define the following quantities: $\bar{p}_s$ is a phase-space point on the surface; P_1 is the probability of a source particle reaching the splitting surface; $g(\bar{p}_s)$ is the conditional pdf of particles that crossed the surface for the first time at $\bar{p}_s$; $w(1,\bar{p}_s)$ is the weight of a particle at the first crossing of the surface at $\bar{p}_s$, distributed with a pdf given by $f_1[w(1,\bar{p}_s)]$. Now, $P_d(\bar{p}_s)$ is the probability of a particle that crossed the splitting surface for the first time at $\bar{p}_s$ to reach the detector region, and w_d is the contribution of that particle at the detector, assuming that the particle reached the splitting surface with unit weight. Let w_d be distributed with pdf $f_d(w_d)$. In these definitions, we have separated the random variable w into a product of two independent parts $w(1,\bar{p}_s)$ and w_d. Given these quantities, the expected D can now be written as

$$D = P_1 \int_s g(\bar{p}_s) d\bar{p}_s P_d(\bar{p}_s) \int_0^\infty w(1,\bar{p}_s) f_1[w(1,\bar{p}_s)] \times dw(1,\bar{p}_s) \int_0^\infty w_d f_d(w_d) dw_d \ . \tag{7}$$

For simple presentation we will omit in each case the dependence on $\bar{p}_s$ and rewrite D as

$$D = \left\langle P_1 P_d \int_0^\infty w(1) f_1[w(1)] dw(1) \times \int_0^\infty w_d f_d(w_d) dw_d \right\rangle_s \ , \tag{8}$$

with the brackets indicating averaging over the splitting surface. With this notation, the second moment can be written as

$$S_1^2 = \left\langle P_1 P_d \int_0^\infty \int_0^\infty w^2(1) w_d^2 f_1[w(1)] f_d(w_d) \times dw(1) dw_d \right\rangle_s \ . \tag{9}$$

On the introduction of splitting, a single independent event will consist of a weight reaching the splitting surface at $\bar{p}_s$, with probability $P_1 g(\bar{p}_s) d\bar{p}_s$ being split into ν particles, from which k will reach the detector and contribute to the total score

$$\eta_\nu = w(1) \frac{[w_d^1 + \ldots w_d^k]}{\nu} \ .$$

The average for all k is thus given by

[15]C. J. EVERETT and EDMOND D. CASHWELL, "Cost of Splitting in Monte Carlo Transport," LA-7189-MS, Los Alamos National Laboratory (1978).

[16]MacDonald and Cashwell (Ref. 17) use pattern recognition for the in-code optimization of the location of a 1:2 phase-space splitting surface. Also, Juzaitis (Ref. 10) applied the second-moment equation to surface splitting in a monokinetic slab model.

[17]JAMES L. MACDONALD and EDMOND D. CASHWELL, "The Application of Artificial Intelligence Techniques to the Acceleration of Monte Carlo Transport Calculations," LA-7475-MS, Los Alamos National Laboratory (1978).

$$\langle \eta_\nu \rangle = \left\langle P_1 \sum_{k=1}^{\nu} \binom{\nu}{k} \frac{P_d^k (1-P_d)^{\nu-k}}{\nu} \int_0^\infty \cdots \int_0^\infty w(1) \right.$$
$$\times \left(\sum_{j=1}^{k} w_d^j \right) f_1[w(1)] f_d(w_d^1)$$
$$\left. \cdots f_d(w_d^k) dw(1) dw_d^1 \cdots dw_d^k \right\rangle_s .$$

Because the w_d^i's are independent and identically distributed, by taking the sum over j out of the integral, we obtain k identical integrals:

$$\langle \eta_\nu \rangle = \left\langle \frac{P_1}{\nu} \int_0^\infty \int_0^\infty w(1) f_1[w(1)] w_d f_d(w_d) dw(1) dw_d \right.$$
$$\left. \times \sum_{k=1}^{\nu} \binom{\nu}{k} k P_d^k (1-P_d)^{\nu-k} \right\rangle_s .$$

Using the general notation

$$\langle w \rangle = \int_0^\infty w f(w) dw$$

and the properties of the average number of successes out of ν trials in a binomial experiment with success probability P_d, we obtain

$$\langle \eta_\nu \rangle = \left\langle P_1 \nu P_d \frac{\langle w(1) \rangle \langle w_d \rangle}{\nu} \right\rangle_s = \langle P_1 P_d \langle w(1) \rangle \langle w_d \rangle \rangle_s = D . \tag{10}$$

The last equality is obtained by comparing with Eq. (8). Thus, the splitting process yields an unbiased estimate of D, a well-known result.

We now calculate the second moment. This will take the form

$$S_\nu^2 = \langle \eta^2 \rangle = \left\langle P_1 \sum_{k=1}^{\nu} \binom{\nu}{k} P_d^k (1-P_d)^{\nu-k} \right.$$
$$\times \int_0^\infty \cdots \int_0^\infty w^2(1)$$
$$\times \frac{\left(\sum_{j=1}^{k} w_d^j \right)^2 f_1[w(1)] \cdot f_d(w_d^1) \cdots f_d(w_d^k)}{\nu^2}$$
$$\left. \times dw(1) dw_d^1 \cdots dw_d^k \right\rangle_s$$
$$= \left\langle P_1 \sum_{k=1}^{\nu} \binom{\nu}{k} P_d^k (1-P_d)^k \right.$$
$$\left. \times \frac{[k \langle w^2(1) \rangle \langle w_d^2 \rangle + k(k-1) \langle w^2(1) \rangle \langle w_d \rangle^2]}{\nu^2} \right\rangle_s$$
$$= \left\langle \frac{P_1 P_d \langle w(1)^2 \rangle \langle w_d^2 \rangle}{\nu} + P_1 P_d^2 \langle w^2(1) \rangle \langle w_d \rangle^2 \right.$$
$$\left. \times \frac{(\nu-1)}{\nu} \right\rangle_s = S_\nu^2 . \tag{11}$$

In Eq. (11) we used the fact that

$$\sum_{k=1}^{\nu} \binom{\nu}{k} P^k (1-P)^{\nu-k} k(k-1) = \nu P^2 (\nu-1) . \tag{12}$$

This can be proved easily from the properties of the binomial distribution. Noting that the dependence on ν is independent of $\bar{p}_s$, it can be taken out of the integration over $\bar{p}_s$ and we can write

$$S_\nu^2 = \frac{\langle P_1 P_d \langle w^2(1) \rangle \langle w_d^2 \rangle \rangle_s}{\nu} + \langle P_1 P_d^2 \langle w^2(1) \rangle \langle w_d \rangle^2 \rangle_s \frac{(\nu-1)}{\nu} . \tag{13}$$

Comparison of the first term with Eq. (9) shows that the coefficient of $1/\nu$ is simply S_1^2 and denoting the second coefficient C we get

$$S_\nu^2 = \frac{S_1^2}{\nu} + C \frac{(\nu-1)}{\nu} . \tag{14}$$

We have thus derived an exact expression for the second moment as a function of the splitting parameter ν.

Some assumptions are inherent in the above model. Though particles may cross a splitting surface any number of times, they are split only on the first crossing. By allowing the particle's weight to be a random variable, rather than unity, biasing methods other than splitting are included. However, if the biasing scheme depends on the splitting parameter (as may be the case with Russian Roulette) and weight cutoff, the weight distribution, and consequently the weight averages, may depend on the splitting parameter. Particles are not allowed to bifurcate in the medium; thus, reactions such as $(n,2n)$ or fission are excluded, except in those cases where it is possible to encounter such reactions by changing the weight rather than creating new tracks. The above limiting conditions apply equally to the n-surface case.

The first term in Eq. (14) is the no-correlation term because it involves only squares of contributions of the same secondary. The no-correlation term is exactly a factor ν smaller than S_1^2 and eventually goes to zero as ν goes to infinity. The second term is the result of cross products of weights of different secondaries. This correlation term decreases the efficiency of the method and results in the second moment having an asymptotic value of C. Intuitively, we note that correlation among secondaries will be small as long as $\nu P_d \ll 1$, in accordance with Eq. (13), because C is smaller than S_1^2 by approximately a factor of P_d. A $1/\nu$ behavior may thus be expected at low values of ν; that is, the first term in the Eq. (13) dominates.

To attain the quality factor, we now need the average time of a source particle. We denote τ as the average time of a source particle without splitting

and τ_1 as the average time of a secondary. The time required to process N source particles will be

$$T_\nu = N\tau + NP_1\tau_1(\nu - 1) = > \tau_\nu = \tau + P_1\tau_1(\nu - 1) \ . \tag{15}$$

Therefore, the quality factor is given by

$$q_\nu = \left[\frac{S_1^2}{\nu} + C\,\frac{(\nu - 1)}{\nu}\right][\tau + P_1\tau_1(\nu - 1)] \ . \tag{16}$$

Consider now the ratio q_ν/q_1, which is the benefit factor, denoted by B_ν. It is the advantage of splitting by ν instead of no splitting; in other words, the time ratio to obtain a given standard deviation. Thus,

$$B_\nu = \frac{q_\nu}{q_1} = \left[\frac{1}{\nu} + d_1\,\frac{(\nu - 1)}{\nu}\right][1 + P_1\beta_1(\nu - 1)] \ ,$$

$$\beta_1 = \frac{\tau_1}{\tau} \ ,$$

and

$$d_1 = \frac{C}{S_1^2} \ . \tag{17}$$

The value of ν, for which B_ν is minimal, is the optimum, ν_{opt}. A useful approximation can be obtained if we assume that both $f_1(w)$ and P_d are independent of $\bar{p}_s$; that is, identical for each point on the surface. This approximation is called the point-surface approximation because it is equivalent to the assumption $g(\bar{p}_s) = \delta(\bar{p}_s - \bar{p}_0)$, $\bar{p}_0$ being a fixed point on the surface. Using this approximation,

$$d_1 = \frac{C}{S_1^2} \cong \frac{P_1P_d^2\langle w^2(1)\rangle\langle w_d\rangle^2}{P_1P_d\langle w^2(1)\rangle\langle w_d^2\rangle} = P_d\,\frac{\langle w_d\rangle^2}{\langle w_d^2\rangle}$$

$$\langle P_1\rangle_s = P_1 = \text{constant}$$

$$\langle P_d\rangle_s = P_d = \text{constant} \ . \tag{18}$$

Differentiating B_ν with respect to ν and equating to zero,

$$\nu_{\text{opt}} = \left[\frac{(d_1 - 1)(P_1\beta_1 - 1)}{d_1P_1\beta_1}\right]^{1/2} \ . \tag{19}$$

Going back to the exact case, we examine B_ν in some special cases. Consider a surface-leakage detector and let the splitting surface coincide with the detector surface. We expect the splitting to have no effect. In that case, $\langle w_d\rangle \equiv 1$, $\langle w_d^2\rangle \equiv 1$, $P_d \equiv 1$, $w(1) = w$, and $P_1 = P_{pd}$, yielding $C = \langle P_{qd}\langle w^2\rangle\rangle_s = S_1^2 = > d_1 = 1$; also $\tau_1 = 0$ yields $\beta_1 = 0$, so that $B_\nu = 1/\nu + (\nu - 1)/\nu \equiv 1$, as expected. If we have a surface source and move the splitting surface to the source, $w(1) = 1$, $w_d = w$, $P_1 = 1$, and $P_d = P_{qd}$. Also $\beta_1 = 1$ because $\tau_1 = \tau$, and

$$B_\nu = \left[\frac{1}{\nu} + \frac{\langle P_{qd}^2\langle w^2\rangle\rangle_s}{\langle P_{qd}\langle w^2\rangle\rangle_s}\,\frac{(\nu - 1)}{\nu}\right](1 + \nu - 1)$$

$$= 1 + \frac{\langle P_{qd}^2\langle w^2\rangle\rangle_s}{\langle P_{qd}\langle w^2\rangle\rangle_s}\,(\nu - 1) \ . \tag{20}$$

In this case, though one might have expected $B_\nu = 1$, instead, $B_\nu \geqslant 1$, which indicates that if $\nu > 1$, splitting is less efficient. However, this is in accordance with the fact that "Batch" estimation has a higher variance than single-particle estimation.[14] Also note that when $\nu = 1$, $B_\nu \equiv 1$ as should be.

In many cases of leakage calculations, especially when absorption probabilities are small, splitting is applied with analog Monte Carlo. Then $w(1) = w_d \equiv 1$, so that

$$B_\nu = \left[\frac{1}{\nu} + \frac{\langle P_d^2\rangle_s}{\langle P_d\rangle_s}\,\frac{(\nu - 1)}{\nu}\right][1 + P_1\beta_1(\nu - 1)] \ .$$

In the point-surface approximation,

$$B_\nu = \left[\frac{1}{\nu} + P_d\,\frac{(\nu - 1)}{\nu}\right][1 + P_1\beta(\nu - 1)]$$

and

$$\nu_{\text{opt}} \cong \left[\frac{(P_d - 1)(P_1\beta_1 - 1)}{P_dP_1\beta_1}\right]^{1/2} \ . \tag{21}$$

Because $\langle P_d^2\rangle_s > \langle P_d\rangle_s^2$, the point-surface approximation causes an overestimation of both B_ν and ν_{opt}. Yet, if $P_d(\bar{p})$ does not vary sharply on the surface, the approximation may be very useful. In the process of the optimization, one may start with a trial ν_1, and after a batch of N_1 source particles, obtain a first estimate of ν_{opt} (ν_2) for N_2 or more source particles by estimating β_1 and using Eq. (21) or (19). Then both d_1 and $(P_1 \cdot \beta_1)$ of Eq. (17) can be estimated by the value of $\hat{B}_{\nu_1}/\hat{B}_{\nu_2}$ and the execution time ratios. The P_1 can be estimated directly in each batch. Note that the parameters appearing in the above discussion, P_1, P_d, $\langle w(1)\rangle$, $\langle w_d\rangle$, etc., are bulk properties of the medium. The accuracy required for d_1 and $(P_1 \cdot \beta)$ is much lower than that required for D, and even a crude estimation yields near-optimum values of $\hat{\nu}_{\text{opt}}$. These aspects are discussed further and demonstrated in Sec. V. Equations (17) and (19) show not only the optimal splitting factor, but the benefit to be expected from the optimal use of splitting.

III. TWO-SURFACE SPLITTING

This case is somewhat more complicated than the one-surface case. It is worthwhile to treat two-surface splitting separately because its derivation contains all the essential features of the general n-surface case and its extension to the general case is straightforward.

We first describe the form of an independent single event with the corresponding pdf for its occurrence. A source particle reaches the first surface ($S1$) at phase-space point $\bar{p}_{S1}$ with weight $w_1(1)$. To write the probability density of this partial event, we define the following quantities, where

P_1 = probability of a source particle to reach the first splitting surface ($S1$)

$g_1(\bar{p}_{S1})$ = conditional pdf of a source particle reaching and crossing $S1$ for the first time at $\bar{p}_{S1}$

$f_1[w(1),\bar{p}_{S1}]$ = conditional pdf of a source particle crossing $S1$ at $\bar{p}_{S1}$ with a weight of $w(1)$.

Note that $\bar{p}_{S1}$ should also appear as an argument in $w(1)$; the omission of this dependence will cause no ambiguity. Using the above definitions, we may write the pdf of the partial event as

$$P_1 \times g_1(\bar{p}_{S1}) \times f_1[w_1(1), \bar{p}_{S1}] \ .$$

Upon crossing $S1$, the particle is split into ν_1 secondary particles, each of weight $w_1(1)/\nu_1$. Of these ν_1 split particles starting at $S1$, $0 \leqslant K^2(1) \leqslant \nu_1$ will reach the second splitting surface ($S2$). Between $S1$ and $S2$ these $K^2(1)$ split particles will accumulate the weights $w_2(1,1), w_2(1,2), \ldots, w_2[1,K^2(1)]$. Each weight is considered as if the particle left $S1$ with unit weight. Therefore, the real weight of a split particle on $S2$ is $w_1(1)w_2(1,i_2)$. So far, each particle reaching $S1$ is identified by a one-dimensional array ($i_1 \equiv 1$); a progeny of that particle reaching $S2$ is identified by a two-dimensional array $(1,i_2)$, $i_2 = 1, \ldots, K^2(1)$. These progenies cross $S2$ at phase-space points $\bar{p}_{S2}^{(1,i_2)}$ with weights $w_2(1,i_2)$. The following definitions apply to that part of the total event, where

$P_2(\bar{p}_{S1})$ = probability that a particle starting at $\bar{p}_{S1}$ will cross the second splitting surface

$g_2[p_{S2}^{(1,i_2)}]$ = conditional pdf that a particle will cross $S2$ at $\bar{p}_{S2}^{(1,i_2)}$

$f_2[w(1,i_2),\bar{p}_{S2}^{(1,i_2)}]$ = conditional pdf that a particle crossing $S2$ at $\bar{p}_{S2}^{(1,i_2)}$ has accumulated weight $w_2(1,i_2)$, having started from surface $S1$ with unit weight.

With the above definitions, the pdf of the partial event between $S1$ and $S2$ can be written as

$$\begin{bmatrix} \nu_1 \\ K^2(1) \end{bmatrix} P_2^{K^2(1)}(\bar{p}_{S1})[1-P_2(\bar{p}_{S1})]^{[\nu_1-K^2(1)]}$$
$$\times g_2[(\bar{p}_{S2}^{(1,1)})] f[w_2(1,1), \bar{p}_{S2}^{(1,1)}]$$
$$\times g_2[\bar{p}_{S2}^{(1,2)}] f_2[w_2(1,2), \bar{p}_{S2}^{(1,2)}] \times \ldots \times g_2\{\bar{p}_{S2}^{[1,K^2(1)]}\}$$
$$\times f_2\{w_2[1,K^2(1)], \bar{p}_{S2}^{[1,K^2(1)]}\}$$
$$= \begin{bmatrix} \nu_1 \\ K^2(1) \end{bmatrix} P_2^{K^2(1)}(\bar{p}_{S1})[1-P_2(\bar{p}_{S1})]^{[\nu_1-K^2(1)]}$$
$$\times \prod_{i_2=1}^{K^2(1)} g_2[\bar{p}_{S2}^{(1,i_2)}] f_2[w_2(1,i_2), \bar{p}_{S1}^{(1,i_2)}] \ ,$$

where

$$\begin{bmatrix} \nu \\ K \end{bmatrix} \equiv \binom{\nu}{K} = \frac{\nu!}{(\nu-K)!K!} \ .$$

Following the same line of thought, each particle $(1,i_2)$ is split on $S2$ into ν_2 particles, from which only $k^d(1,i_2)$ reach the detector and contribute $w_d(1,i_2,i_d)$, $i_d = 1, \ldots, K^d(1,i_2)$. Each particle is identified now by a three-dimensional vector $(1,i_2,i_d)$, uniquely defining that particle as the i_d'th progeny of the particle $(1,i_2)$, which is the i_2'th progeny of (1). The weight $w(1,i_2,i_d)$ is accumulated assuming unit weight on $S2$, so that the total contribution to D from a given branch $[(1), (1,i_2), (1,i_2,i_d)]$ is $w_1(1)w_2(1,i_2)w_d(1,i_2,i_d)$ (Fig. 2). The following definitions are introduced, where

$P_d[\bar{p}_{S2}^{(1,i_2)}]$ = probability of a particle emitted from $\bar{p}_{S2}^{(1,i_2)}$ on $S2$ reaching the detector region

$f_d[w_d(1,i_2,i_d)]$ = conditional pdf for a particle reaching the detector to contribute a weight $w_d(1,i_2,i_d)$, having left surface $S2$ with unit weight.

The probability density of the third and last part of the single history is

$$\begin{bmatrix} \nu_2 \\ K^d(1,i_2) \end{bmatrix} P_d^{K^d(1,i_2)}[\bar{p}_{S2}^{(1,i_2)}]\{1-P_d[\bar{p}_{S2}^{(1,i_2)}]\}^{[\nu_2-K^d(1,i_2)]}$$
$$\times \prod_{i_d=1}^{K^d(1,i_2)} f_d[w_d(1,i_2,i_d)] \ .$$

The contribution of a single independent event may now be written as

$$\eta = \frac{w_1(1)}{\nu_1}\left(\frac{w_2(1,1)}{\nu_2}\{w_d(1,1,1) + \ldots + w_d[1,1,K^d(1,1)]\}\right)$$
$$+ \left(\frac{w_2(1,2)}{\nu_2}\{w_d(1,2,1) + \ldots + w_d[1,2,K^d(1,2,)]\}\right) \ldots \ldots$$
$$+ \ldots + \left[\frac{w_2[1,K^2(1)]}{\nu_2}\left(w_d[1,K^2(1),1] + \ldots w_d\{1,K^2(1),K^d[1,K^2(1)]\}\right)\right]$$

$$= \sum_{i_2=1}^{K^2(1)} \frac{w_1(1)}{\nu_1} \sum_{i_d=1}^{K^d(1,i_2)} \frac{w_2(1,i_2)}{\nu_2} \cdot w_d(1,i_2,i_d)$$

$$= \sum_{i_2=1}^{K^2(1)} \sum_{i_d=1}^{K^d(1,i_2)} \frac{w_1(1)w_2(1,i_2)w_d(1,i_2,i_d)}{\nu_1\nu_2} \quad . \tag{22}$$

The probability density of such an event is given by

$$\rho(\eta) = P_1 \times g_1(\bar{p}_{S1}) f_1[w(1),\bar{p}_{S1}] \begin{bmatrix} \nu_1 \\ K^2(1) \end{bmatrix} p_2^{K^2(1)}(\bar{p}_{S1}) \times \{1 - P_2(p_{S1})^{[\nu_1 - K^2(1)]}\} \times \prod_{j_2=1}^{K^2(1)} \left(g_2[\bar{p}_{S2}^{(1,j_2)}] f_2[w_2(1,j_2), \bar{p}_{S2}^{(1,j_2)}] \times \begin{bmatrix} \nu_2 \\ K^d(1,j_2) \end{bmatrix} P_d^{K^d(1,j_2)}[\bar{p}_{S2}^{(1,j_2)}] \times \{1 - P_d[\bar{p}_{S2}^{(1,j_2)}]\}^{[\nu_2 - K^d(1,j_2)]} \times \prod_{j_d=1}^{K^d(1,j_2)} f_d[w_d(1,j_2,j_d)] \right) \quad . \tag{23}$$

To obtain the r'th moment of η, η^r should be multiplied by $\rho(\eta)$; integration should be performed from zero to infinity on each weight and splitting surface $\bar{p}_{Si}$. Each j_2 summation should be performed over $K^d(1,j_2)$ from one to ν_2, and on $K^2(1)$ from one to ν_1.

To treat the first moment, we multiply η of Eq. (22) with $\rho(\eta)$ of Eq. (23) and perform the averaging process described above. This can be presented as

$$\langle \eta \rangle = \int_0^\infty dw_1(1) \int_{S1} d\bar{p}_{S1} \sum_{K^2(1)=1}^{\nu} P_1 \cdot g_1(\bar{p}_{S1}) \times f_1[w_1(1), \bar{p}_{S1}] \begin{bmatrix} \nu_1 \\ K^2(1) \end{bmatrix} P_2^{K^2(1)}(\bar{p}_{S1}) \times [1 - P_2(\bar{p}_{S1})]^{[\nu_1 - K^2(1)]} \cdot \prod_{j_2=1}^{k^2(1)} \int_{S2} d\bar{p}_{S2}^{(1,j_2)} \times \int_0^\infty dw_2(1,j_2) g_2[\bar{p}_{S1}^{(1,j_2)}] \times f_2[w_2(1,j_2), \bar{p}_{S2}^{(1,j_2)}] \sum_{K^d(1,j_2)=1}^{\nu_2} \begin{bmatrix} \nu_2 \\ K^d(i,j_2) \end{bmatrix} \times P_d^{K^d(1,j_2)}[\bar{p}_{S2}^{(1,j_2)}] \times \{1 - P_d[\bar{p}_{S2}^{(1,j_2)}]\}^{[\nu_2 - K^d(1,j_2)]} \cdot \prod_{j_d=1}^{K^d(1,j_2)} \times \int_0^\infty dw_d(1,j_2,j_d) f_d[w_d(1,j_2,j_d)] \cdot \eta \quad . \tag{24}$$

We first note that $\rho(\eta)$ contains a product of the pdf's of *all* the partial weights in the event, whereas η contains a sum of terms each of which contains a product of the weights in one branch only, for example, $w_1(1)w_2(1,3)w_d(1,3,2)$. Thus, if we multiply the product of the pdf's by η, we get a sum of terms for which each term contains a product of a subset of the weights multiplied by their corresponding pdf's and by the rest of the pdf's without a corresponding weight.

When performing the integration over the weights, all the pdf's that are not multiplied by a corresponding weight will integrate to unity. Those multiplied by a weight will yield the average weight. Thus,

$$\sum_{i_2=1}^{K^2(1)} \sum_{i_d=1}^{K^d(1,i_2)} \langle w_1(\bar{p}_{S1}) \rangle \cdot \langle w_2[\bar{p}_{S2}^{(1,i_2)}] \rangle \cdot \frac{\langle w_d \rangle}{\nu_1\nu_2} \quad . \tag{25}$$

In the averages, dependence on the splitting-surface phase-space point is explicitly expressed as related to the dependence of the pdf used in averaging on that phase-space point. Because Eq. (25) does not depend on i_d, it can be written as

$$\sum_{i_2=1}^{K^2(1)} \langle w_1(\bar{p}_{S1}) \rangle \langle w_2(\bar{p}_{S2}^{(1,i_2)}) \rangle \frac{\langle w_d \rangle}{\nu_1\nu_2} K^d(1,i_2) \quad . \tag{26}$$

In Eq. (24) all the terms containing f_1, f_2, f_d, or the integrals over the weights, are omitted because they have been used in the averaging of expression (26).

The summation over $K^d(1,j_2)$ and multiplication over j_2 now reads

$$\prod_{j_2=1}^{K^2(1)} \left(\sum_{K^d(1,j_2)=1}^{\nu_2} g_2[\bar{p}_{S2}^{(1,j_2)}] \begin{bmatrix} \nu_2 \\ K^d(1,j_2) \end{bmatrix} \times P_d^{K^d(1,j_2)}[\bar{p}_{S2}^{(1,j_2)}] \{1 - P_d[\bar{p}_{S2}^{(1,j_2)}]\}^{[\nu_2 - K^d(1,j_2)]} \right) \times \sum_{i_2=1}^{K^2(1)} \langle w_1(\bar{p}_{S1}) \rangle \langle w_2[\bar{p}_{S2}^{(1,i_2)}] \rangle \frac{\langle w_d \rangle}{\nu_1\nu_2} K^d(1,i_2) \quad . \tag{27}$$

We use

$$B[K^d(1,j_2)] = \begin{bmatrix} \nu_2 \\ K_2^d(1,j_2) \end{bmatrix} P_d^{K^d(1,j_2)}[\bar{p}_{S2}^{(1,j_2)}] \times \{1 - P_d[\bar{p}_{S2}^{(1,j_2)}]\}^{[\nu - K^d(1,j_2)]} \quad , \tag{28}$$

to reflect the probability of having $K^d(1,j_2)$ successes out of ν_2 trials in a binomial experiment with success probability $P_d(\bar{p}_{S2}^{(1,j_2)})$. We denote

$$\alpha(1,i_2) = \langle w_1(\bar{p}_{S1}) \rangle \langle w_2[\bar{p}_{S2}^{(1,i_2)}] \rangle \langle w_d \rangle / \nu_1\nu_2 \quad .$$

With this notation, Eq. (27) can be written as

$$\sum_{i_2=1}^{K^2(1)} \alpha(1,i_2) \prod_{j_2=1}^{K^2(1)} \left\{ \sum_{K^d(1,j_2)=0}^{\nu_2} g_2[\bar{p}_{S2}^{(1,j_2)}] B[K^d(1,j_2)] \right\} \times K^d(1,i_2) \quad . \tag{29}$$

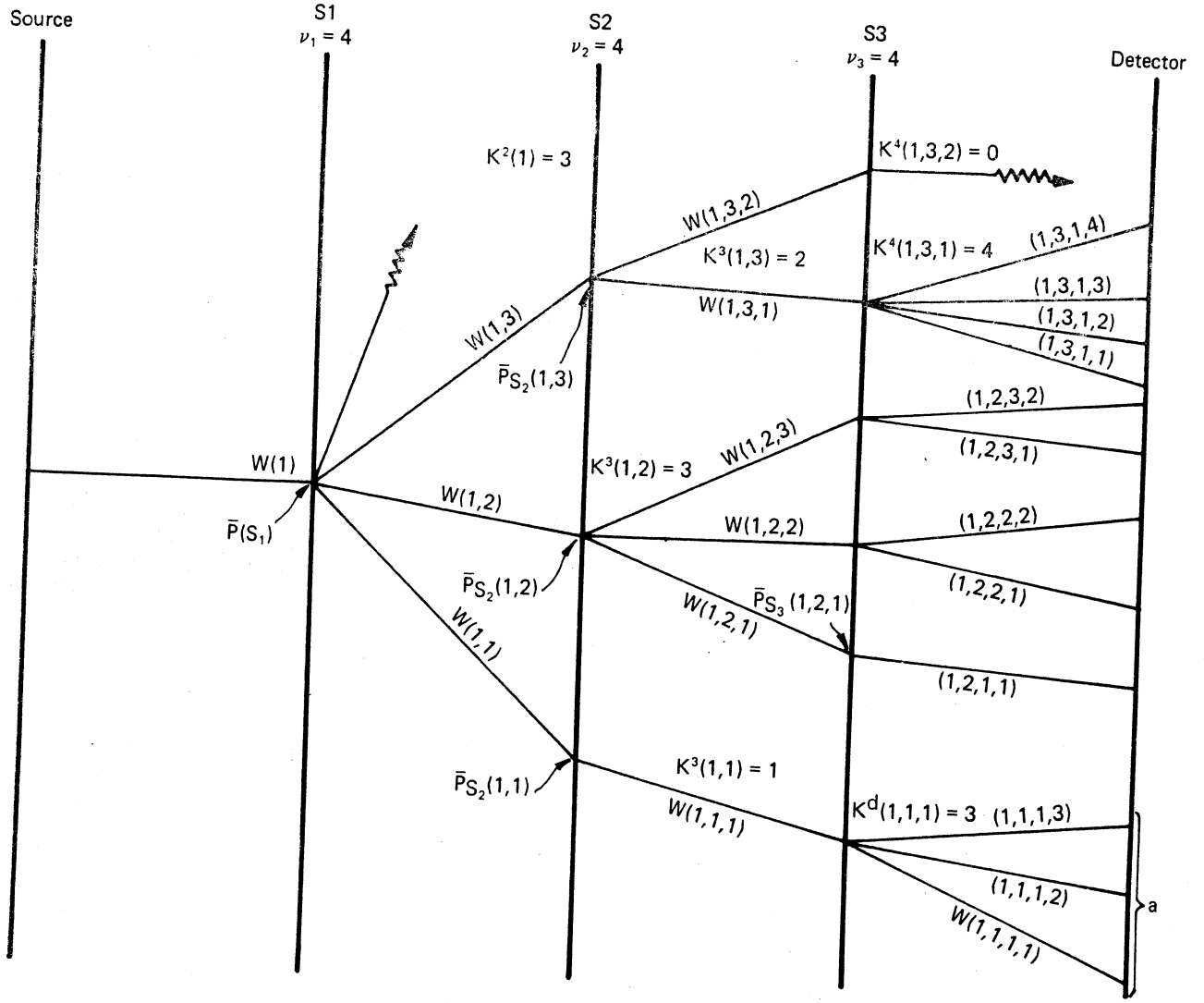


Fig. 2. Example of splitting event and related parameters.

Consider now the summation over $K^d(1,j_2)$. For $j_2 = 1$, we sum over $K^d(1,1)$ from zero to ν_2; if $i_2 \neq 1$, the summation is done over $B[K^d(1,1)]$ in the product and yields unity (sum of binomial probabilities with any number of successes). Thus, for every $j_2 \neq i_2$, the summation yields unity in the product, independent of $\bar{p}_{S2}^{(1,j_2)}$. There will be only one term for each i_2, for which $i_2 = j_2$, and the summation[18] over this term will give $P_d[\bar{p}_{S2}^{(1,i_2)}]\cdot\nu_2$. Thus, from Eq. (29),

$$\sum_{i_2=1}^{K^2(1)} \alpha(1,i_2)\nu_2 P_d[\bar{p}_{S2}^{(1,i_2)}] \prod_{j_2=1}^{K^2(1)} g_2[\bar{p}_{S2}^{(1,j_2)}] \quad . \tag{30}$$

[18]Note that the multiplication over j_2 does not apply to $K^d(1,i_2)$. However, for $j_2 = i_2$ the summation over $K^d(1,j_2)$ applies to $K^d(1,i_2)$.

Using Eq. (24), we integrate over all $\bar{p}_{S2}^{(1,j_2)}$. When $j_2 \neq i_2$, every term in the product integrates to unity. When $j_2 = i_2$, we average over the second splitting surface and obtain

$$\frac{1}{\nu_1\nu_2} \sum_{i_2=1}^{K^2(1)} [\langle w_1(\bar{p}_{S1})\rangle \nu_2 \langle\langle w_2\rangle \times P_d\rangle_{S2} \langle w_d\rangle]$$

$$= \frac{K^2(1)}{\nu_1} \langle w_1(\bar{p}_{S1})\rangle \langle\langle w_2\rangle P_d\rangle \langle w_d\rangle P_d\rangle_{S2} \langle w_d\rangle \quad , \tag{31}$$

where

$$\langle\langle w_2\rangle P_d\rangle_{S2} = \int_{S2} \int_0^\infty w_2 f_2(w_2,\bar{p}_{S2}) P_d(\bar{p}_{S2}) g_2(p_{S2}) \times dw_2 d\bar{p}_{S2} \quad . \tag{32}$$

Returning to Eq. (24), we have already performed the integrations over the weight and over $S2$ and the summation over $K^d(1,j_2)$; we are left with

$$\langle\eta\rangle = \int_{S1} d\bar{p}_{S1} \sum_{K^2(1)=0}^{\nu_1} P_1 \cdot g_1(\bar{p}_{S1}) B[K^2(1)] K^2(1) \times \frac{\langle w_1(p_{S1})\rangle \langle\langle w_2\rangle p_d\rangle_{S2}}{\nu_1} \langle w_d\rangle \ , \quad (33)$$

where $B[K^2(1)]$ is the same shorthand notation used in Eq. (28), with ν_1 and $P_2(\bar{p}_{S1})$ replacing ν_2, $P_d(\bar{p}_{S2})$. The summation over $K^2(1)$ involves only the product $B[K^2(1)] \times K^2(1)$ and yields $\nu_1 \times P_2(\bar{p}_{S1})$. Finally, we obtain

$$\begin{aligned}\langle\eta\rangle &= P_1 \langle P_2 \times \langle w_1\rangle\rangle_{S1} \langle\langle w_2\rangle P_d\rangle_{S2} \langle w_d\rangle \\ &= P_1 \int_0^\infty \int_{S2} \int_0^\infty \int_{S1} \int_0^\infty P_2(\bar{p}_{S1}) w_1 f_1(w_1, \bar{p}_{S1}) \\ &\quad \times g_1(\bar{p}_{S1}) w_2 f_2(w_2, \bar{p}_{S2}) P_d(\bar{p}_{S2}) g_2(\bar{p}_{S2}) \\ &\quad \times w_d f_d(w_d) dw_1 d\bar{p}_{S1} dw_2 d\bar{p}_{S2} dw_d \equiv D \ . \end{aligned} \quad (34)$$

In the second moment,

$$\eta^2 = \left[\sum_{i_2=1}^{K^2(1)} \sum_{i_d=1}^{K^d(1,i_2)} \frac{w_1(1) \times w_2(1,i_2) \times w_d(1,i_2,i_d)}{\nu_1 \cdot \nu_2} \right]^2 . \quad (35)$$

We will divide η^2 into three terms. The first contains unmixed squares, that is, squares of contributions from the same branch particle. This term has the form

$$\eta^2_{\text{unmixed}} = \sum_{i_2=1}^{K^2(1)} \sum_{i_d=1}^{K^d(1,i_2)} \times \frac{w_1^2(1) \times w_2^2(1,i_2) \times w_d^2(1,i_2,i_d)}{\nu_1^2 \nu_2^2} \ . \quad (36)$$

Comparison of Eqs. (36) and (22) shows that when averaging $\langle\eta^2\rangle$, the treatment of η^2_{unmixed} will follow exactly the same route as in $\langle\eta\rangle$. It will yield the same result, with w_i^2 replacing w_i for every i, and with additional division by $\nu_1\nu_2$ because η^2_{unmixed} contains $(1/\nu_1\nu_2)^2$. Thus,

$$\langle\eta^2_{\text{unmixed}}\rangle = \frac{P_1 \langle P_2 \langle w_1^2\rangle\rangle_{S1} \langle\langle w_2^2\rangle P_d\rangle_{S2} \langle w_d^2\rangle}{\nu_1\nu_2} \equiv \frac{S_1^2}{\nu_1\nu_2} \ . \quad (37)$$

This is the no-correlation term and, as in the one-surface case, neglecting correlation between secondaries brings about a reduction in the second moment by a factor equaling the total splitting of a source particle reaching the detector, $\nu_1\nu_2$. We expect that correlation terms will moderate this reduction and yield a finite asymptotic value for the second moment.

The next term contains products of contributions from particle branches whose tracks are identical up to surface $S2$ (Fig. 2). This term can be written

$$\eta^2_{S2} = 2 \sum_{i_2=1}^{K^2(1)} \frac{w_1^2(1) w_2^2(1,i_2)}{(\nu_1\nu_2)^2} \sum_{i_d=1}^{[K^d(1,i_2)-1]} \sum_{i'_d=1+i_d}^{K^d(1,i_2)} \times w_d(1,i_2,i_d) w_d(1,i_2,i'_d) \ . \quad (38)$$

We repeat the process started at Eq. (24) with η^2_{S2} replacing η. The multiplication and integration with the pdf's of the weights will now result in

$$a_1 = \sum_{i_2=1}^{K^2(1)} \langle w_1^2 \bar{p}_{S1}\rangle \langle w_2^2[\bar{p}_{S2}^{(1,i_2)}]\rangle \langle w_d\rangle^2 K^d(1,i_2) \times [K^d(1,i_2) - 1] \ . \quad (39)$$

Note that for w_d we obtain $\langle w_d\rangle^2$ and not $\langle w_d^2\rangle$, because the averaging is done for two independent, identically distributed random variables $w_d(1,i_2,i_d)$ and $w_d(1,i_2,i'_d)$ $(i_d \neq i'_d)$. We may now repeat the process of Eqs. (27) and (28) and through the same process reach the parallel of Eq. (29) that will now be

$$a_2 = \sum_{i_2=1}^{K^2(1)} \alpha_{S2}(1,i_2) \prod_{j_2=1}^{K^2(1)} \sum_{K^d(1,j_2)=1}^{\nu_2} g_2[\bar{p}_{S2}^{(1,j_2)}] \times B[K^d(1,j_2)] K^d(1,i_2) \cdot [K^d(1,i_2) - 1] \quad (40)$$

with

$$\alpha_{S2}(1,i_2) = \langle w_1^2(p_{S1})\rangle \langle w_2^2[\bar{p}_{S2}^{(1,i_2)}]\rangle \langle w_d\rangle^2/(\nu_1\nu_2)^2 \ , \quad (41)$$

and $K^d(K^d - 1)$ replacing K^d of Eq. (29). Using the same arguments leading to Eqs. (30), we obtain

$$a_2 = \sum_{i_2=1}^{K^2(1)} \alpha_{S2}(1,i_2) P_d^2[\bar{p}_{S2}^{(1,i_2)}] \nu_2(\nu_2 - 1) \times \prod_{j_2=1}^{K^2(1)} g_2[\bar{p}_{S2}^{(1,j_2)}]/(\nu_1\nu_2)^2 \ . \quad (42)$$

By integrating a_2 over $\bar{p}_{S2}^{(1,j_2)}$, $j_2 = 1, \ldots, K^2(1)$, we obtain

$$\begin{aligned} a_3 &= \sum_{i_2=1}^{K^2(1)} \nu_2(\nu_2 - 1) \langle w_1^2(\bar{p}_{S1})\rangle_{S1} \langle w_2^2\rangle \times P_d^2\rangle_{S2} \\ &\quad \times \langle w_d\rangle^2/(\nu_2\nu_1)^2 \\ &= \frac{(\nu_2 - 1)}{\nu_1^2\nu_2} \langle w_1^2(\bar{p}_{S1})\rangle_{S1} \langle\langle w_2^2\rangle p_d^2\rangle_{S2} \langle w_d\rangle^2 \cdot K^2(1) \ . \end{aligned} \quad (43)$$

By reinserting a_3 into the remainder of the averaging process, we obtain the analog of Eq. (33), with

$$\frac{(\nu_2 - 1)}{\nu_1^2\nu_2} \langle w_1^2\rangle \langle\langle w_2^2\rangle P_d^2\rangle \langle\langle w_2^2\rangle P_d^2\rangle_{S2} \langle w_d\rangle^2$$

replacing

$$\frac{\langle w_1\rangle}{\nu_1} \langle\langle w_2\rangle P_d\rangle_{S2} \langle w_d\rangle \ .$$

The summation over $K^2(1)$ and integration over $\bar{p}_{S1}$ are now identical to those of Eqs. (33) and (34), and we finally obtain

$$\langle \eta^2_{S2} \rangle = \frac{P_1 \langle P_2 \times \langle w_1^2 \rangle \rangle_{S1} \langle\langle w_2^2 \rangle \times P_d^2 \rangle_{S2} \langle w_d \rangle^2 (\nu_2 - 1)}{\nu_1 \nu_2} . \tag{44}$$

Comparison of Eqs. (44) and (37) indicates that (a) introduction of correlations from surface $S2$ eliminates the $1/\nu_2$ dependence and, at the same time, (b) the coefficient of that correlation term is smaller by approximately a factor P_d. The same phenomenon was observed in the one-surface case. Thus, at small values of ν_1, ν_2, the uncorrelated term dominates; at large values of ν_1, ν_2, it approaches zero and the correlated terms dominate.

The third and last term of η^2 consists of products of contributions from particles whose tracks are identical only up to $S1$. A pattern develops in which taking the correlation to $S1$ will eliminate the $1/\nu_1$ dependence, while also reducing the coefficient by a factor $\cong P_2$. This term has the form

$$\eta^2_{S1} = \frac{2}{\nu_1^2 \nu_2^2} \sum_{i_2=1}^{[K^2(1)-1]} \sum_{i_2'=i_2+1}^{K^2(1)} \sum_{i_d=1}^{K^d(1,i_2)} \sum_{i_d'=1}^{K^d(1,i_2')} \times w_1^2(1) w_2(1,i_2) w_2(1,i_2') \times w_d(1,i_2,i_d) w_d(1,i_2',i_d') . \tag{45}$$

We repeat the process of averaging indicated by Eq. (24), integrating η^2_{S1} with the weights of pdf's:

$$b_1 = \frac{2}{\nu_1^2 \nu_2^2} \sum_{i_2=1}^{[K^2(1)-1]} \sum_{i_2'=i_2+1}^{K^2(1)} \times \underbrace{\langle w_1^2(\bar{p}_{S1}) \rangle \langle w_2[\bar{p}_{S2}^{(1,i_2)}] \rangle \langle w_2[\bar{p}_{S2}^{(1,i_2')}] \rangle \langle w_d \rangle^2}_{\alpha_{S1}(i_2,i_2')} \times K^d(1,i_2) K^d(1,i_2') . \tag{46}$$

Summing this expression over $K^d(1,j_2)$ and taking a product over j_2 as in Eq. (29),

$$b_2 = \frac{2}{\nu_1^2 \nu_2^2} \sum_{i_2=1}^{[K^2(1)-1]} \sum_{i_2'=i_2+1}^{K_2^2(1)} \alpha_{S1}(i_2,i_2') \times \prod_{j_2=1}^{K^2(1)} g[\bar{p}_2^{(1,j_2)}]_{S2} \sum_{K^d(1,j_2)=1}^{\nu_2} B[K^d(1,j_2)] \times K^d(1,i_2) K^d(1,i_2') . \tag{47}$$

Unlike Eq. (29), here, when the summation is done over $K^d(1,j_2)$, there will be two terms for which $j_2 = i_2$ and $j_2 = i_2'$. Therefore, the result of the sum for each product over j_2 is $\nu_2^2 P_d[\bar{p}_{S2}^{(1,i_2)}] P_d[\bar{p}_{S2}^{(1,i_2')}]$, so that

$$b_2 = \frac{2}{\nu_1^2} \sum_{i_2=1}^{K^2(1)-1} \sum_{i_2'=i_2+1}^{K^2(1)} \alpha_{S1}(i_2,i_2') P_d[\bar{p}_{S2}^{(1,i_2)}] P_d[\bar{p}_{S2}^{(1,i_2')}] \times \prod_{j_2=1}^{K^2(1)} g_2[\bar{p}_{S2}^{(1,j_2)}] . \tag{48}$$

By integrating b_2 over all $\bar{p}_{S2}$'s,

$$b_3 = \langle w_1^2(\bar{p}_{S1}) \rangle \langle\langle w_2 \rangle \cdot P_d \rangle_{S2}^2 \langle w_d \rangle^2 \frac{K^2(1)[K^2(1)-1]}{\nu_1^2} ,$$

and as in Eq. (33),

$$\langle \eta^2_{S1} \rangle = \int_{S1} d\bar{p}_{S1} \sum_{K^2(1)=0}^{\nu_1} P_1 g_1(\bar{p}_{S1}) B[K^2(1)] b_3$$

$$= P_1 \langle\langle w_1^2 \rangle P_2^2 \rangle_{S1} \langle\langle w_2 \rangle \cdot P_d \rangle_{S2}^2 \langle w_d \rangle^2 \frac{(\nu_1 - 1)}{\nu_1}$$

$$= c_1 \frac{(\nu_1 - 1)}{\nu_1} . \tag{49}$$

Thus, we can now write the second moment for two-surface splitting as

$$\langle \eta^2 \rangle = S_2^2(\nu_1, \nu_2) = \langle \eta^2_{\text{unmixed}} \rangle + \langle \eta^1_{S2} \rangle + \langle \eta^2_{S1} \rangle = \frac{S_1^2}{\nu_1 \nu_2} + \frac{c_2(\nu_2 - 1)}{\nu_1 \nu_2} + \frac{c_1(\nu_1 - 1)}{\nu_1} , \tag{50}$$

where c_2 and c_1 can be deduced easily from Eqs. (44) and (49). In the point-surface approximation, assuming that P_2, P_d, and the pdf's of the weights are independent of the point on the surface, then

$$\langle \hat{\eta}^2 \rangle \cong \frac{S_1^2}{\nu_1 \nu_2} + \frac{P_1 P_2 P_d^2 \langle w_1^2 \rangle \langle w_2^2 \rangle \langle w_d \rangle^2 (\nu_2 - 1)}{\nu_1 \nu_2} + \frac{P_1 P_2^2 P_d^2 \langle w_1^2 \rangle \langle w_2 \rangle^2 \langle w_d \rangle^2 (\nu_1 - 1)}{\nu_1} . \tag{51}$$

Taking the correlation back to S_1 resulted in reduction of the $1/\nu_1$ dependence to an asymptotic value of c_1 smaller than c_2 by approximately a factor of P_2.

In the above model, we assume that the pdf's of the weights depend only on the point at which the particle branch crosses the surface. Thus, $f_2(w_2)$ depends on $\bar{p}_{S2}^{(1,j_2)}$ only. Then $f_2\{[w_2^{(1,j_2)}]\bar{p}_{S1}^{(1,j_2)}\}$ must be some average over the surface $S1$, or f_2 is also dependent on the crossing point at $S1$ and $f_2(w_2, \bar{p}_{S2}, \bar{p}_{S1})$. In the same way, $f_d(w_d)$ is either an average over $S2$ (and a nontrivial average), or it depends on $\bar{p}_{S2}^{(1,j_2)}$. Taking the more elaborate dependence into account, however, will not alter Eq. (51), but merely change the form of the coefficients c_1 and c_2 so that the averaging over $S1$ and $S2$ cannot be separated. For example, c_1 of Eq. (49) will become $[P_1 \langle\langle w_1^2 \rangle P_2^2 \langle (\langle w_2 \rangle P_d)^2 \langle w_d \rangle^2 \rangle_{S2} \rangle_{S1}]$. The same approach applies to the more general n-surface case.

The calculation of c_2 and c_1 in the course of a Monte Carlo run is prohibitively difficult because averaging must be performed over the $g_1(\bar{p}_{Si})$'s. However, c_2 and c_1 can be estimated from Eq. (51), where all the quantities are "bulk properties" that are easier to calculate than D itself. Therefore, $S_2^2(\nu_1,\nu_2)/S_1^2 = r_2(\nu_1,\nu_2)$ gives us

$$r_2(\nu_1,\nu_2) = \frac{1}{\nu_1\nu_2} + \frac{d_2(\nu_2-1)}{\nu_1\nu_2} + \frac{d_1(\nu_1-1)}{\nu_1} \quad . \tag{52}$$

In the point-surface approximation

$$S_1^2 = P_1P_2P_d\langle w_1^2\rangle\langle w_2^2\rangle\langle w_d^2\rangle \ ,$$

resulting in

$$d_1 = P_2P_d \frac{\langle w_2\rangle^2}{\langle w_2^2\rangle} \cdot \frac{\langle w_d\rangle^2}{\langle w_d^2\rangle} \tag{53a}$$

and

$$d_2 = P_d \frac{\langle w_d\rangle^2}{\langle w_d^2\rangle} \ . \tag{53b}$$

We realize that if two values of $r_2(\nu_1,\nu_2)$ are known, then d_1 and d_2 can be calculated by using three initial batches for three different pairs of (ν_1,ν_2). However, after the first batch, d_1 and d_2 can be estimated from Eq. (53) by using quantities obtainable in the course of the run. The next two batches are already done in a near-optimum zone by use of Eq. (52). This procedure will be further demonstrated in the numerical example.

If τ_1 and τ_2 are the average times required to process a particle starting from $S1$ and $S2$, respectively, the time to process N source particles will be

$$T(\nu_1,\nu_2) = N\tau + NP_1(\nu_1-1)\tau_1 + N\langle P_2\rangle_{S1}\nu_1(\nu_2-1)\tau_2 \ ,$$

and the time ratio will be

$$T_r(\nu_1\nu_2) = \frac{T_N(\nu_1,\nu_2)}{T_N(1,1)} = [1+\gamma_1(\nu_1-1)+\gamma_2\nu_1(\nu_2-1)] \ , \tag{54}$$

where

$$\gamma_1 = P_1\beta_1 \ (\beta_1 = \tau_1/\tau)$$
$$\gamma_2 = \langle P_2\rangle_{S1}\beta_2 \ (\beta_2 = \tau_2/\tau) \ .$$

Both γ_1 and γ_2 can also be estimated easily from the times obtained in the same three batches that are used for d_1 and d_2.

Finally, the functional expression of the benefit factor is given by

$$B_2(\nu_1,\nu_2) = r_2(\nu_1,\nu_2)T_r(\nu_1,\nu_2) = \left[\frac{1}{\nu_1\nu_2} + \frac{d_2(\nu_2-1)}{\nu_1\nu_2} + \frac{d_1(\nu_1-1)}{\nu_1}\right] \times [1+\gamma_1(\nu_1-1)+\gamma_2\nu_1(\nu_2-1)] \ . \tag{55}$$

IV. n-SURFACE SPLITTING

Following the conventions of the preceding section, we now adopt the following notations and definitions:

$(1,i_2,1_3,\ldots,i_m)$
= m-dimensional array uniquely identifying a split particle reaching the m'th splitting surface. This particle is a progeny of the particle $(1,i_2,\ldots,i_{m-1})$ that reached surface S_{m-1} and was split there into ν_{m-1} particles from which $K^m(1,i_2,i_3,\ldots,i_{m-1})$ reached surface S_m.

$w_m(1,i_1,\ldots,i_m)$
= additional weight accumulated by the particle reaching S_m, assuming that the particle left surface S_{m-1} with unit weight

$f_m[w_m(1,\ldots,i_m),\bar{p}_{Sm}^{(1,\ldots,i_m)}]$
= conditional pdf where $\bar{p}_{Sm}^{(1,\ldots,i_m)}$ is the phase-space point at which the particle crosses S_m

$P_m[\bar{p}_{S(m-1)}]$
= probability of a particle generated at $\bar{p}_{S(m-1)}$ to cross surface S_m

$g_m(\bar{p}_{Sm})$
= conditional distribution of a particle to cross surface S_m at $\bar{p}_{Sm}$.

As stated before, the index addressing the particles that reach the detector region is (i_d). With the above definitions, which are extensions of the definitions of the preceding section, we can write the contribution, or score, of a single independent source particle history with n splitting surfaces and with ν_m splitting on S_m as

$$\eta = \sum_{i_2=1}^{K^2(1)} \sum_{i_3=1}^{K^3(1,i_2)} \sum_{i_4=1}^{K^4(1,i_2,i_3)} \cdots \sum_{i_n=1}^{K^n(1,i_2,\ldots,i_{n-1})} \times \sum_{i_d=1}^{K^d(1,\ldots,i_n)} = \frac{w_1(1)w_2(1,i_2)w_3(1,i_2,i_3)\ldots w_d(1,i_2,\ldots,i_n,i_d)}{\nu_1\nu_2\nu_3\ldots\nu_n} \ . \tag{56}$$

The pdf of the above contribution, though lengthy, is merely an extension of Eq. (23) and can be written as

$$\rho(\eta) = P_1 g_1(\bar{p}_{S1}) \times f_1[w_1(1), \bar{p}_{S1}] \begin{bmatrix} \nu_1 \\ K^2(1) \end{bmatrix} P_2^{K^2(1)}(\bar{p}_{S1})[1 - P_2(\bar{p}_{S1})]^{[\nu_1 - K^2(1)]}$$

$$\times \prod_{j_2=1}^{K^2(1)} g_2[\bar{p}_{S2}^{(1,j_2)}] \cdot f_2[w_2(1,j_2), \bar{p}_{S2}^{(1,j_2)}] \begin{bmatrix} \nu_2 \\ K^3(1,j_2) \end{bmatrix} P_3^{K^3(1,j_2)}[\bar{p}_{S2}^{(1,j_2)}]$$

$$\times \{1 - P_3[\bar{p}_{S2}^{(1,j_2)}]\}^{[\nu_2 - K^3(1,j_2)]} \times \prod_{j_3=1}^{K^3(1,j_2)} g_3^3[\bar{p}_{S3}^{(1,j_2,j_3)}]$$

$$\times f_3[w_3(1,j_2,j_3), \bar{p}_{S3}^{(1,j_2,j_3)}] \times \begin{bmatrix} \nu_3 \\ K^4(1,j_2,j_3) \end{bmatrix} P_4^{K^4(1,j_2,j_3)}[\bar{p}_{S3}^{(1,j_2,j_3)}]$$

$$\times \{1 - P_4[\bar{p}_{S3}^{(1,j_2,j_3)}]\}^{[\nu_3 - K^4(1,j_2,j_3)]} \prod_{j_4=1}^{K^4(1,j_2,j_3)} \cdots$$

$$\cdots \times \prod_{j_{n-1}=1}^{K^{n-1}(1,\ldots,j_{n-2})} g_{n-1}[\bar{p}_{S(n-1)}^{(1,\ldots,j_{n-1})}] f_{n-1}[w_{n-1}(1,j_2,\ldots,j_{n-1}), \bar{p}_{S(n-1)}^{(1,\ldots,j_{n-1})}]$$

$$\times \begin{bmatrix} \nu_{n-1} \\ K^n(1,j_2,\ldots,j_{n-1}) \end{bmatrix} P_n^{K^n(1,\ldots,j_{n-1})}[\bar{p}_{S(n-1)}^{(1,\ldots,j_{n-1})}] \times \{1 - P_n[\bar{p}_{S(n-1)}^{(1,\ldots,j_{n-1})}]\}^{[\nu_{n-1} - K^n(1,\ldots,j_{n-1})]}$$

$$\times \prod_{j_n=1}^{K^n(1,\ldots,j_{n-1})} g_n[\bar{p}_{Sn}^{(1,\ldots,j_n)}] f_n[w_n(1,\ldots,j_n), \bar{p}_{Sn}^{(1,\ldots,j_n)}] \times \begin{bmatrix} \nu_n \\ K^d(1,\ldots,j_n) \end{bmatrix}$$

$$\times P_d^{K^d(1,\ldots,j_n)}[\bar{p}_{Sn}^{(1,\ldots,j_n)}] \times \{1 - P_d[\bar{p}_{Sn}^{(1,\ldots,j_n)}]\}^{[\nu_n - K^d(1,\ldots,j_n)]} \times \prod_{j_d=1}^{K^d(1,\ldots,j_n)} f_d[w_d(1,j_2,\ldots,j_n,j_d)]$$

$$= P_1 g_1(\bar{p}_{S1}) f_1[w_1(1), \bar{p}_{S1}] \begin{bmatrix} \nu_1 \\ K^2(1) \end{bmatrix} P_2^{K^2(1)}(\bar{p}_{S1})[1 - P_2(\bar{p}_{S1})]^{[\nu_1 - K^2(1)]}$$

$$\times \prod_{l=2}^{n} \prod_{j_l=1}^{K^l(1,\ldots,j_{l-1})} g_l[\bar{p}_{Sl}^{(1,\ldots,j_l)}] f_l[w_l(1,\ldots,j_l), \bar{p}_{Sl}^{(1,\ldots,j_l)}]$$

$$\times \begin{bmatrix} \nu_l \\ K^{l+1}(1,j_2,\ldots,j_l) \end{bmatrix} P_{l+1}^{K^{l+1}(1,\ldots,j_l)}[\bar{p}_{Sl}^{(1,\ldots,j_l)}] \cdot \{1 - P_{l+1}[\bar{p}_{Sl}^{(1,\ldots,j_l)}]\}^{[\nu_l - K^{l+1}(1,\ldots,j_l)]}$$

$$\times \prod_{j_d=1}^{K^d(1,\ldots,j_n)} f_d[w_d(1,\ldots,j_n,j_d)] \quad , \quad n+1 \equiv d \ . \tag{57}$$

We adopt the shorthand notation

$$B[K^l(1,\ldots,j_{l-1})] = \begin{bmatrix} \nu_{l-1} \\ K^l(1,\ldots,j_{l-1}) \end{bmatrix} P_l^{K^l(1,\ldots,j_{l-1})}[\bar{p}_{S(l-1)}^{(1,\ldots,j_{l-1})}]$$
$$\times \{1 - P_l[\bar{p}_{S(l-1)}^{(1,\ldots,j_{l-1})}]\}^{[\nu_{l-1} - K^l(1,\ldots,j_{l-1})]} \ , \tag{58}$$

which is the probability that of ν_{l-1} particles emitted at $\bar{p}_{S(l-1)}^{(1,\ldots,j_{l-1})}$, exactly $K^l(1,\ldots,j_{l-1})$ particles will reach surface *Sl*.

We recall the useful relations

$$\sum_{K^l(1,\ldots,j_{l-1})=0}^{\nu_{l-1}} B[K^l(1,\ldots,j_{l-1})] \equiv 1 \tag{58a}$$

and

$$\sum_{K^l(1,\ldots,j_{l-1})=1}^{\nu_l} B[K^l(1,\ldots,j_{l-1})]K^l(1,\ldots,j_{l-1}) = \nu_{l-1}P_l[\bar{p}_{S(l-1)}^{(1,\ldots,j_{l-1})}] \tag{58b}$$

and

$$\sum_{K^l(1,\ldots,j_{l-1})=1}^{\nu_{l-1}} B[K^l(1,\ldots,j_{l-1})]K^l(1,\ldots,j_{l-1})[K^l(1,\ldots,j_{l-1})-1] = \nu_{l-1}(\nu_{l-1}-1)P_l^2[\bar{p}_{S(l-1)}^{(1,\ldots,j_{l-1})}] \ . \tag{58c}$$

We skip the derivation of the first moment, which is identical to the derivation of the no-correlation term of the second moment and can thus easily be repeated, and look directly at the second moment. The η^2 can be subdivided into partial sums so that the first sum contains squares of contributions from the same particle's track (or branch); this η^2_{unmixed} will lead to the uncorrelated term. The second partial sum contains products of contributions from particles whose tracks are identical up to (and only up to) the n'th surface, η^2_{Sn}. In this part, the $1/\nu_n$ dependence will be removed. In general, η^2_{Sl} is the partial sum containing products of contributions from particles whose tracks are identical up to the l'th surface (Sl).

Let us start with η^2_{unmixed}. This process of averaging extends that discussed in Sec. III and contains (a) integration over all the weights, for all possible arrangement of indices, (b) integration over all surface phase-space points, and (c) summation over every $K^l(1,\ldots,j_{l-1})$ for every set $(1,\ldots,j_{l-1})$ from 1 to ν_{l-1}. This averaging process is expressed in the form

$$\begin{aligned}\langle\rho(\eta)\cdot\chi\rangle = &\int_{S1} d\bar{p}_{S1}\int_0^\infty dw_1(1)P_1 g_1(\bar{p}_{S1})f_1[w_1(1),\bar{p}_{S1}]\sum_{k^2(1)=1}^{\nu_1}\begin{bmatrix}\nu_1\\K^2(1)\end{bmatrix}P_2^{K^2(1)}(\bar{p}_{S1})[1-P_2(\bar{p}_{S1})]^{[\nu_1-K^2(1)]}\\
&\times\prod_{l=2}^{n}\left\{\prod_{j_l=1}^{K^l(1,\ldots,j_{l-1})}\left\{\int_{Sl}d\bar{p}_{Sl}^{(1,\ldots,j_l)}\int_0^\infty dw_l(1,\ldots,j_l)g_l[\bar{p}_{Sl}^{(1,\ldots,j_l)}]\right.\right.\\
&\times f_l[w_l(1,\ldots,j_l),\bar{p}_{Sl}^{(1,\ldots,j_l)}]\left(\sum_{K^{l+1}(1,j_2,\ldots,j_l)=1}^{\nu_l}P_{l+1}^{K^{l+1}(1,\ldots,j_l)}[\bar{p}_{Sl}^{(1,\ldots,j_l)}]\right.\\
&\left.\left.\times\{1-P_{l+1}[\bar{p}_{Sl}^{(1,\ldots,j_l)}]\}^{[\nu_l-K^{l+1}(1,\ldots,j_l)]}\right)\prod_{j_d=1}^{K^d(1,\ldots,j_n)}\int_0^\infty dw_d(1,\ldots,j_d)\right.\\
&\left.\times f_d[w_d(1,\ldots,j_d)]\cdot\chi\right\}\Bigg\}\ ,\quad n+1\equiv d\ ,\end{aligned} \tag{59}$$

where the products over the j_l's are those appearing in $\rho(\eta)$ and χ is any quantity to be averaged with $\rho(\eta)$.

Then, η^2_{unmixed} is given by

$$\eta^2_{\text{unmixed}} = \sum_{i_2=1}^{K^2(1)}\sum_{i_3=1}^{K^3(1,i_2)}\cdots\sum_{i_d=1}^{K^d(1,\ldots,i_n)}\frac{[w_1(1)\ldots w_d(1,\ldots,i_d)]^2}{(\nu_1\ldots\nu_n)^2}\ .$$

In Eq. (59) we have the product of all the pdf's of the various weights. We first apply the integration over the weights on η^2_{unmixed} and obtain

$$a_1 = \sum_{i_2=1}^{K^2(1)}\cdots\sum_{i_n=1}^{K^n(1,\ldots,i_{n-1})}\frac{\langle w_1^2(p_{S1})\rangle\langle w_2^2[\bar{p}_{S2}^{(1,i_2)}]\rangle\ldots\langle w_d^2\rangle}{(\nu_1\ldots\nu_n)^2}K^d(1,i_2,\ldots,i_n)\ .$$

By inserting a_1 into Eq. (59) where the integration over the weights was already performed, we execute the product over j_n and the summation over $K^d(1,\ldots,j_n)$. Summing over $K^d(1,\ldots,j_n)$, Eq. (57a) will apply for all $j_n \neq i_n$. We find $\nu_n \times P_d[\bar{p}_{Sn}^{(1,\ldots,i_n)}]$ only for $(1,\ldots,j_n)=(1,\ldots,i_n)$ by using Eq. (57b). We integrate over $\bar{p}_{Sn}^{(1,\ldots,j_n)}$ again, obtaining unity for the product over j_n because the integration is done over normalized g_n, except for $(1,\ldots,j_n)\equiv(1,\ldots,i_n)$, where we obtain $\langle\langle w_n^2\rangle P_d\rangle_{Sn}$. At this stage, the product over j_n is concluded and because nothing depends on i_n,

$$a_2 = \sum_{i_2=1}^{K^2(1)} \cdots \sum_{i_{n-2}=1}^{K^{n-1}(1,\ldots,i_{n-2})} \times \frac{\langle w_1(\bar{p}_{S1})\rangle\langle w_2^2[\bar{p}_{S2}^{(1,i_n)}]\rangle \cdots \langle\langle w_n^2\rangle P_d\rangle_{Sn}}{\nu_1^2\nu_2^2 \cdots \nu_{n-1}^2\nu_n} \times K^n(1,\ldots,i_{n-1})\langle w_d^2\rangle \ .$$

The a_2 is calculated by Eq. (59), with index l ranging from 2 to $(n-1)$.

On a_2 we now apply the multiplication over j_{n-1} with the corresponding summation over $K^n(1,j_2,\ldots,j_{n-1})$ and integration over $\bar{p}_{S(n-1)}^{(1,\ldots,j_{n-1})}$. The sum over $K^n(1,\ldots,j_{n-1})$ with $B[K^n(1,\ldots,j_{n-1})]$ will yield unity [Eq. (57a)]; except for the case where $(1,\ldots,j_{n-1}) = (1,\ldots,i_{n-1})$, which gives $\nu_{n-1} \times P_n[\bar{p}_{S(n-1)}^{(1,\ldots,i_{n-1})}]$. Integration over $\bar{p}_{S(n-1)}^{(1,\ldots,j_{n-1})}$ yields unity; again, except for $(1,\ldots,j_{n-1}) = (1,\ldots,i_{n-1})$ where we get $\langle\langle w_{n-1}^2\rangle \cdot P_n\rangle_{S(n-1)}$. Thus,

$$a_3 = \sum_{i_2=1}^{K^2(1)} \cdots \sum_{i_{n-2}=1}^{K^{(n-2)}(1,\ldots,i_{n-2})} \times \frac{\langle w_1^2(\bar{p}_{S1})\rangle \cdots \langle\langle w_{n-1}^2\rangle P_n\rangle_{S(n-1)}\langle\langle w_n^2\rangle P_d\rangle_{Sn}\langle w_d^2\rangle}{\nu_1^2 \cdots \nu_{n-2}^2\nu_{n-1}\nu_n} \times K^{(n-1)}(1,\ldots,i_{n-1}) \ .$$

This process repeats, reversing in j_l; at each stage, the product over j_l, with the summation over $K^{l+1}(1,j_2,\ldots,j_l)$ and integration over $\bar{p}_{Sl}^{(1,\ldots,j_l)}$, yields $\langle w_l^2[\bar{p}_{Sl}^{(1,\ldots,i_l)}]\rangle$ to become $\langle\langle w_l^2\rangle P_{l+1}\rangle_{Sl}$ and leave no dependence on i_l. After executing the product over any j_l, we can execute the product over j_{l-1}, with corresponding summation over K^l and integration over $\bar{p}_{S(l-1)}$, applied to

$$a_{n-l+1} = \sum_{i_2=1}^{K^2(1)} \cdots \sum_{i_{l-1}=1}^{K^{l-1}(1,\ldots,i_{l-2})} \frac{\langle w_1^2(\bar{p}_{S1})\rangle \cdots \langle w_{l-1}^2[\bar{p}_{S(l-1)}^{(1,\ldots,i_{l-1})}]\rangle\langle w_l^2\rangle P_{l+1}\rangle_{Sl} \cdots \langle\langle w_n^2\rangle P_d\rangle_{Sn}\langle w_d^2\rangle}{\nu_1^2 \cdots \nu_{l-1}^2\nu_l \cdots \nu_n} K_l(1,\ldots,i_{l-1}) \ . \tag{60}$$

Recall that a_{n-l+1} describes the propagation of the average as j_l reverses toward j_1. Putting $l = 1$ into Eq. (60), we immediately obtain the required average:

$$a_n = \langle \eta_{\text{unmixed}}^2 \rangle = \frac{P_1\langle\langle w_1^2\rangle P_2\rangle_{S1}\langle\langle w_2^2\rangle P_3\rangle_{S2} \cdots \langle\langle w_n^2\rangle P_d\rangle_{Sn}\langle w_d^2\rangle}{\nu_1\nu_2 \cdots \nu_n} = \frac{S_1^2}{\nu_1 \cdots \nu_n} \ . \tag{61}$$

We see that the unmixed term gives the expected $1/\nu_1 \ldots \nu_n$ dependence. The correlation terms reduce that dependence until particles of common track only up to $S1$ are considered and yield an asymptotic constant as $\nu_1 \ldots \nu_n$ increases.

The term $\eta_{Sl}^2 (l = 1,\ldots,n)$ contains products of contributions from particles whose track is identical up to and only up to the l'th splitting surface. Thus

$$\eta_{Sl}^2 = 2 \cdot \sum_{i_2=1}^{K^2(1)} \cdots \sum_{i_{l-1}=1}^{K^{l-1}(1,\ldots,i_{l-2})} \sum_{i_l=1}^{K^l(1,\ldots,i_{l-1})} \sum_{i_{l+1}=1}^{[K^{l+1}(1,\ldots,i_l)-1]} \sum_{i'_{l+1}=i_{l+1}+1}^{K^{l+1}(1,\ldots,i_l)} \sum_{i_{l+2}=1}^{K^{l+2}(1,\ldots,i_{l+1})} \sum_{i'_{l+2}=1}^{K^{l+2}(1,\ldots,i_l,i'_{l+1})}$$

$$\cdots \sum_{i_d=1}^{K^d(1,\ldots,i_l,i_{l+1},\ldots,i_n)} \sum_{i'_d=1}^{K^d(1,\ldots,i_l,i'_{l+1},\ldots,i'_n)} [w_1^2(1) \ldots w_l^2(1,\ldots,i_l)]$$

$$\times [w_{l+1}(1,\ldots,i_{l+1})w_{l+1}(1,\ldots,i'_{l+1})\ w_{l+2}(1,\ldots,i_l,i_{l+1},i_{l+2})w_{l+2}(1,\ldots,i_l,i'_{l+1},i'_{l+2})$$

$$\times \ldots \times w_d(1,\ldots,i_d)w_d(1,\ldots,i_l,i'_{l+1},\ldots,i'_d)]/(\nu_1 \ldots \nu_n)^2 \ . \tag{62}$$

We now substitute Eq. (62) into the averaging process of Eq. (59), and follow a process similar to that used for η_{unmixed}^2. The first step is integration over the pdf's of the weights. This process turns η_{Sl}^2 into

$$a_1 = 2 \sum_{i_2=1}^{K^2(1)} \sum_{i_l=1}^{K^l(1,\ldots,i_{l-1})} \sum_{i_{l+1}=1}^{[K^{l+1}(1,\ldots,i_l)-1]} \sum_{i'_{l+1}=i_{l+1}+1}^{K^{l+1}(1,\ldots,i_l)} \cdots \sum_{i_d=1}^{K^d(1,\ldots,i_n)} \sum_{i'_d=1}^{K^d(1,\ldots,i_l,i'_{l+1},\ldots,i'_n)}$$

$$\times \langle w_1^2(\bar{p}_{S1})\rangle \ldots \times \langle w_l^2[\bar{p}_{Sl}^{(1,\ldots,i_l)}]\rangle\langle w_{l+1}[\bar{p}_{S(l+1)}^{(1,\ldots,i_{l+1})}]\rangle\langle w_{l+1}[\bar{p}_{S(l+1)}^{(1,\ldots,i_l,i'_{l+1})}]\rangle \times \ldots \times \langle w_d\rangle^2/(\nu_1 \ldots \nu_n)^2 \ .$$

This expression does not depend on i_d or i'_d, so it can be written as

$$a_1 = 2 \sum_{i_2=1}^{K^2(1)} \cdots \sum_{i_l=1} \sum_{i_{l+1}=1} \sum_{i'_{l+1}=i_{l+1}} \cdots \sum_{i_n=1}^{K^n(1,\ldots,i_{n-1})} \sum_{i'_n=1}^{K^n(1,\ldots,i_l,i'_{l+1},\ldots,i_{n-1})}$$
$$\times \langle w_1^2(\bar{p}_{S1})\rangle \ldots \langle w_d\rangle^2 K^d(1,\ldots,i_n) K^d(1,\ldots,i_l,i'_{l+1},\ldots,i'_n)/(\nu_1 \ldots \nu_n)^2 \ .$$

As before, we apply on a_1 the product over j_n, with the summation over $K^d(1,\ldots,j_n)$ and integration over the n'th splitting surface phase-space points. In the summation over $K^d(1,j_2,\ldots,j_n)$, Eq. (57a) applies except when $(1,j_2,\ldots,j_n) = (1,i_2,\ldots,i_n)$ and when $(1,j_2,\ldots,j_n) = (1,\ldots,i_l,i'_{l+1}\ldots i'_n)$. Both cases will occur because $(1,j_2,\ldots,j_n)$ scans all possible branches of the random walk. From the two cases of matching indices and by using Eq. (57b), we obtain

$$\nu_n P_d[\bar{p}_{Sn}^{(1,i_2,\ldots,i_n)}]\,\nu_n P_d[\bar{p}_{Sn}^{(1,i_2,\ldots,i_l,i'_{l+1},\ldots,i'_n)}] \ .$$

Integration over $\bar{p}_{Sn}^{(1,\ldots,i_n)}$ for every possible $(1,\ldots,j_n)$ will leave the expression independent of i_n and i'_n, and will thus result in

$$a_2 = 2 \sum_{i_2=1}^{K^2(1)} \cdots \sum_{i_l}^{K^l(1,\ldots,i_{l-1})} \sum_{i_{l+1}=1}^{[K^{l+1}(1,\ldots,i_l)-1]} \sum_{i'_{l+1}=i_{l+1}+1}^{K^{l+1}(1,\ldots,i_l)} \cdots \sum_{i'_{n-1}=1}^{K^{n-1}(1,\ldots,i_l,i_{l+1},\ldots,i_{n-2})} \sum_{i'_{n-1}=1}^{K^{n-1}(1,\ldots,i_l,i'_{l+1},\ldots,i_{n-2})}$$
$$\times \langle w_1^2(\bar{p}_{S1})\rangle \ldots \langle w_{n-1}[\bar{p}_{S(n-1)}^{(1,i_2,\ldots,i_{n-1})}]\rangle\langle w_{n-1}[\bar{p}_{S(n-1)}^{(1,\ldots,i_l,i'_{l+1},\ldots,i'_{n-1})}]\rangle$$
$$\times \langle\langle w_n\rangle P_d\rangle_{Sn}^2 \langle w_d\rangle^2 K^n(1,i_2,\ldots,i_{n-1}) K^n(1,\ldots,i_l,i'_{l+1},\ldots,i'_{n-1})/(\nu_1 \ldots \nu_{n-1})^2 \ .$$

Note that the $1/\nu_n$ dependence is removed.

This process will be repeated as we go backward in applying the product over j_m, where at each stage

$$\langle w_m[\bar{p}_{S(m+1)}^{(1,\ldots,i_m)}]\rangle\langle w_m[\bar{p}_{S(m+1)}^{(1,\ldots,i'_m)}]\rangle$$

is transformed into

$$\langle\langle w_m\rangle P_{m+1}\rangle_{Sm}^2 \nu_m^2 \times K^m(1,\ldots,i_m) K^m(1,\ldots,i_l,i'_{l+1},\ldots,i'_m) \ ,$$

which eliminates the ν_m^{-2} dependence. This process continues until we reach the product over j_{l+1}, which is applied to

$$a_{n-l} = 2 \sum_{i_2=1}^{K^2(1)} \cdots \sum_{i_l=1}^{K^l(1,\ldots,i_{l-1})} \sum_{i_{l+1}=1}^{[K^{l+1}(1,\ldots,i_l)-1)]} \sum_{i'_{l+1}=i_{l+1}+1}^{K^{l+1}(1,\ldots,i_l)} \langle w_1^2(\bar{p}_{S1})\rangle \ldots \langle w_l^2[\bar{p}_{Sl}^{(1,\ldots,i_l)}]\rangle\langle w_{l+1}[\bar{p}_{S(l+1)}^{(1,\ldots,i_{l+1})}]\rangle$$
$$\times \langle w_{l+1}[\bar{p}_{S(l+1)}^{(1,\ldots,i_l,i'_{l+1})}]\rangle\langle\langle w_{l+2}\rangle P_{S(l+3)}\rangle_{S(l+2)}^2 \cdots \frac{\langle\langle w_n\rangle P_d\rangle_{Sn}^2 \langle w_d\rangle^2 K^{l+2}(1,\ldots,i_{l+1}) K^{l+2}(1,\ldots,i_l,i'_{l+1})}{(\nu_l \ldots \nu_{l+1})^2} \ .$$

With summation over $K^{l+2}(1,\ldots,j_{l+1})$, only two terms will not yield unity; $(1,\ldots,j_{l+1}) = (1,\ldots,i_{l+1})$ and $(1,\ldots,j_{l+1}) = (1,\ldots,i_l,i'_{l+1})$. The final result will be independent of either i_{l+1} or i'_{l+1}; however, because the summation limits of i_{l+1}, i'_{l+1} are different than those previously encountered,

$$a_{n-l+1} = \sum_{i_2=1}^{K^2(1)} \cdots \sum_{i_l=1}^{K^l(1,\ldots,i_{l+1})} \langle w_1^2(\bar{p}_{S1})\rangle \ldots \langle w_l^2[\bar{p}_{Sl}^{(1,\ldots,i_l)}]\rangle \langle\langle w_{l+1}\rangle P_{l+2}\rangle_{S(l+1)}^2 \langle\langle w_{l+2}\rangle P_{l+3}\rangle_{S(l+2)}^2 \ldots \langle\langle w_n\rangle P_d\rangle^2$$
$$\times \frac{\langle w_d^2\rangle[K^{l+1}(1,\ldots,i_l)-1] \times K^{l+1}(1,\ldots,i_l)}{(\nu_1 \ldots \nu_l)^2} \ .$$

On a_{n-l+1} we will apply the product over j_l with the summation over $K^{l+1}(1,j_2,\ldots,j_l)$ and integration over Sl. For every j_l such that $(1,\ldots,j_l) \neq (1,\ldots,i_l)$, the summation over K^{l+1} will yield unity [compare with Eq. (57a)].

However, in the one instance where $(1,\ldots,j_l) = (1,\ldots,i_l)$, Eq. (57c) applies and the result will be

$$a_{n-l+2} = \sum_{i_2+1}^{K^2(1)} \cdots \sum_{i_{l-1}}^{K^{l-1}(1,\ldots,i_{l-2})} \langle w^2(\bar{p}_{S1})\rangle \ldots \langle w_{l-1}^2[\bar{p}_{S(l-1)}^{(1,\ldots,i_l-1)}]\rangle\langle\langle w_l^2\rangle P_{l+1}^2\rangle_{Sl} \times \langle\langle w_{l+1}\rangle P_{l+2}\rangle_{S(l+1)} \ldots \langle\langle w_n\rangle P_d\rangle_{Sn}^2 \langle w_d\rangle^2 \times K^l(1,\ldots,i_{l-1}) \frac{1}{(\nu_1 \ldots \nu_{l-1})^2}\left(\frac{\nu_l - 1}{\nu_l}\right) .$$

From this stage to the final summation over $K^2(1)$ and integration over $\bar{p}_{S1}$, the process is identical to that of η^2_{unmixed}, concluding

$$a_l = \langle \eta_{Sl}^2\rangle = P_1[\langle\langle w_1^2\rangle P_2\rangle_{S1} \ldots \langle\langle w_{l-1}^2\rangle P_l\rangle_{S(l-1)}] \times \langle\langle w_l^2\rangle P_{l+1}^2\rangle_{Sl} \times [\langle\langle w_{l+1}\rangle P_{l+2}\rangle_{S(l+1)}^2 \ldots \langle\langle w_n\rangle P_d\rangle^2\langle w_d\rangle^2] \frac{1}{(\nu_1 \ldots \nu_{l-1})}\left(\frac{\nu_l - 1}{\nu_l}\right)$$

(see Ref. 19) . (63)

The second moment of a general n-splitting-surface Monte Carlo scheme is given by

$$S_n^2(\nu_1, \ldots, \nu_n) = \langle \eta^2_{\text{unmixed}}\rangle + \sum_{l=1}^{n} \langle \eta_{Sl}^2\rangle , \quad (64)$$

where $\langle \eta^2_{\text{unmixed}}\rangle$ is given by Eq. (61), and $\langle \eta_{Sl}^2\rangle$ by Eq. (63).

The general behavior expected is now confirmed. The uncorrelated term is linear in all transfer probabilities and goes to zero as $\nu_i \to \infty$ $(i = 1, \ldots, n)$. The first correlated term (a_n), which accounts for correlations from the n'th surface only, is bilinear in P_d only and is asymptotically constant as $\nu_n \to \infty$:

$$\langle \eta_{Sn}^2\rangle = P_1\left(\prod_{i=1}^{n-1} \frac{\langle\langle w_i^2\rangle P_{i+1}\rangle_{Si}}{\nu_i}\right)\langle\langle w_n^2\rangle P_d^2\rangle_{Sn}\langle w_d\rangle^2\left(\frac{\nu_n - 1}{\nu_n}\right) . \quad (65)$$

The asymptotic value of $S_n^2(\nu_1, \ldots, \nu_n)$ is the coefficient of $\langle \eta_{S1}^2\rangle$ given by

$$E_1 = P_1\langle\langle w_1^2\rangle P_2^2\rangle_{S1} \times \prod_{i=2}^{n} (\langle\langle w_i\rangle P_{i+1}\rangle_{Si}^2)\langle w_d\rangle^2 , \quad n+1 \equiv d . \quad (66)$$

The ratio $S_n^2(\nu_1, \ldots, \nu_n)/S_1^2$ will be denoted by $r_n(\nu_1, \ldots, \nu_n)$ and can be written in the form

$$r_n(\nu_1, \ldots, \nu_n) = \frac{S_n^2}{S_1^2} = \frac{1}{\nu_1 \ldots \nu_n} + \frac{d_n}{\nu_1 \ldots \nu_{n-1}}\frac{\nu_n - 1}{\nu_n} + \frac{d_{n-1}}{\nu_1 \ldots \nu_{n-2}}\frac{\nu_{n-1} - 1}{\nu_{n-1}} + \ldots + d_1\frac{\nu_1 - 1}{\nu_1} . \quad (67)$$

In the point-surface approximation using Eqs. (63) and (61),

$$d_l \cong (P_{l+1}P_{l+2} \ldots P_d)\frac{\langle w_{l+1}\rangle^2}{\langle w_{l+1}^2\rangle}\frac{\langle w_{l+2}\rangle^2}{\langle w_{l+2}^2\rangle} \ldots \frac{\langle w_d\rangle^2}{\langle w_d^2\rangle} , \quad l = 1, \ldots, n , \quad n+1 \equiv d$$

$$= \prod_{i=l+1}^{n+1\equiv d} P_1\frac{\langle w_i\rangle^2}{\langle w_i^2\rangle} . \quad (68)$$

The equations obtained for $n = 2$ can now be derived as a special case of Eqs. (68) and (63). The term $r_n(\nu_1, \ldots, \nu_n)$ requires knowledge of n coefficients $(d_l$'s) that can be determined if n values of $r_n(\nu_1, \ldots, \nu_n)$ are known. This process will require $n + 1$ calculations with different values of the ν_i's; also Eq. (68) can be used to estimate the coefficient. The quantities involved in that estimation are bulk properties that can be tallied during the Monte Carlo calculation.

The time required to process N source particles can be written as

$$T_n(\nu_1, \ldots, \nu_n) = N\tau + NP_1(\nu_1 - 1)\tau_1 + NP_1\langle P_2\rangle_{S1}\nu_1(\nu_2 - 1)\tau_2 + NP_1\langle P_2\rangle_{S1}\langle P_3\rangle_{S2}\nu_1\nu_2(\nu_3 - 1)\tau_3 + \ldots + NP_1\langle P_2\rangle_{S1} \ldots \langle P_n\rangle_{S(n-1)}\nu_1 \ldots \nu_{n-1}(\nu_n - 1)\tau_n . \quad (69)$$

where τ_i is the average time per secondary, starting on the i'th surface. The time ratio $T_r(\nu_1, \ldots, \nu_n)$ is

$$T_r(\nu_1, \ldots, \nu_n) = \frac{T_n(\nu_1, \ldots, \nu_n)}{T_1(1)} = [1 + P_1\beta_1(\nu_1 - 1) + P_1\langle P_2\rangle_{S1}\nu_1(\nu_2 - 1)\beta_2 \ldots + \ldots + P_1\langle P_2\rangle_{S1}\langle P_3\rangle_{S2} \ldots \langle P_n\rangle_{S(n-1)}\nu_1 \ldots \nu_{n-1}(\nu_n - 1)\beta_n]$$
$$= [1 + g_1(\nu_1 - 1) + g_2\nu_1(\nu_2 - 1) + \ldots + g_n\nu_1\nu_2 \ldots \nu_{n-1}(\nu_n - 1)] . \quad (70)$$

The general expression for the benefit factor is given as

$$B_n(\nu_1, \ldots, \nu_n) = r_n(\nu_1, \ldots, \nu_n) \times T_r(\nu_1, \ldots, \nu_n) . \quad (71)$$

[19] Recall that $f_\ell[w_\ell, \bar{p}_{S\ell}]$ is assumed to depend only on $\bar{p}_{S\ell}$, the point of crossing of the surface. If we let f_ℓ depend on both $\bar{p}_{S\ell}$ and $\bar{p}_{S(\ell-1)}$, the coefficient of $(\nu_\ell - 1)/\nu \cdot 1/(\nu \ldots \nu)$ in a_ℓ will be $\langle w_1^2\rangle P_2\langle\langle w_2^2\rangle P_3\langle \ldots \langle\langle w_{\ell-1}^2\rangle P_\ell\langle\langle w_\ell^2\rangle P_{\ell+1}^2\langle(\langle w_{\ell+1}\rangle P_{\ell+1})^2 \times \langle \ldots \langle(\langle w_n\rangle P_d)^2\langle w_d\rangle^2\rangle_{Sn}\rangle_{S(n-1)}\rangle_{S(n-2)} \ldots \rangle_{S2}\rangle_{S1}$. In P-S approximation, Eq. (68) is valid and, in general, the functional form displayed in Eq. (67) is preserved.

The term $T_r(\nu_1, \ldots, \nu_n)$ contains n unknowns (g_i's). However, these unknowns can be obtained in the same $n + 1$ calculations from which the d_l's are obtained.

V. NUMERICAL RESULTS

The following numerical results were obtained for four simple test problems.

V.A. Problem 1

A homogeneous cylinder of x_{det} = 10-cm length and 15-cm radius is considered. Four energy groups are assumed and the source is located at the $x = 0$ plane, emitting particles normally and uniformly distributed in all energy groups. The detector is the leakage current through the x_{det} = 10-cm-plane surface. Table I shows cross sections of the four groups with a transfer probability matrix.

Table II presents some basic numerical results obtained from the Monte Carlo runs. The splitting surface is the plane surface $x_{\text{sp}} = 5$ cm. The P_1 and P_d are approximately two and three orders of magnitude larger than D; thus, their calculation is easier than that of D. The P_1 is obtained by dividing by N_p the number of histories reaching the splitting surface (N_1) for the first time, and P_d is obtained by dividing by N_1 the number of particles reaching the detector surface (N_d). Initially, the average $\langle P_d \rangle_{S1}$ is obtained; P_1 and P_d are by-products of the calculation, requiring negligible additional time.

TABLE I

Particle Transfer Matrix (Probabilities)

Group	Σ_t (cm^{-1})	Σ_s/Σ_t	Into Group 1	2	3	4
1	0.6	1	0.25	0.25	0.25	0.25
2	0.9	$\frac{2}{3}$	0	0.25	0.25	0.5
3	1.2	0.5	0	0	0.25	0.75
4	1.5	0.4	0	0	0	1

Experimental estimates of S^2 are obtained by using the square of the PRSD for each ν and the experimental quality factor [q_{exp} as $(\text{PRSD})^2 T$]. Filled circles in Fig. 3 represent values of the experimental variance ratio $(S_\nu^2/S^2)_{\text{exp}}$ as functions of ν. The statistical nature of these results is illustrated by $\nu = 10$, $(S_{10}^2/S_1^2)_{\text{exp}} = 0.083$, well below the minimum possible value of $\frac{1}{10}$. The theoretical variance $r_1(\nu)$ ratio was calculated in two ways: (a) the point-surface (P-S) approximation (open circles) uses Eq. (18) for d_1. In this case, $\langle w_d \rangle = \langle w_d^2 \rangle \equiv 1$ so that $d_1 = P_d$, yielding an underestimation of the variance ratio and its asymptotic value; this is a result of replacing the second moment of P_d over the splitting surface by the square of the average and (b) the value $(S_{1000}^2/S_1^2)_{\text{exp}}$ was used to calculate $d_1 = 3.663 \times 10^{-3}$, yielding values that closely follow the experimental results. All the results are of a statistical nature and contain large statistical errors. For $\nu = 1$ the error is 27.7% and the statistical error relevant to Fig. 3 is the fourth moment.

Figure 4 shows results for the benefit factors of the above three cases. In Eq. (17), β_1 was derived from T_{400}/T (5000 histories), yielding $\beta_1 = 0.65$, and $B(\nu)$ was calculated from Eq. (17). While $B(\nu)$ derived from d_1 follows quite accurately $B_{\nu(\text{exp})}$, the P-S approximation results in an overestimation of the benefit. Yet optimum ν_{opt} obtained from the P-S approximation [using Eq. (19)] from all the cases $10 \leqslant \nu \leqslant 1000$ was found to be in the range $250 < \nu_{\text{opt}} < 300$ (263 from $\nu = 10$ and 294 from $\nu = 1000$), as seen in Fig. 4. This is a near-optimum range in which the splitting is more efficient than analog Monte Carlo by a factor of $\cong 35$. An important result is that values of ν_{opt} derived from samples not larger than 10% of the samples sizes of Table II (N_p) were also in the range $200 < \nu_{\text{opt}} < 310$. For

TABLE II

Numerical Results for Problem 1: Homogeneous Cylinder with Leakage Detector

ν Splitting	Detector Response, $D \pm$ PRSD (%)	Source Particles Used, $N_p \times 10^{-3}$	T (s)	$P_1 \times 10^2$	$P_d \times 10^4$
0	$1.757 \times 10^{-5} \pm 27.8\%$	740	3073	1.845	9.54
50	$2.228 \times 10^{-5} \pm 6.1\%$	290	1917	1.835	12.14
100	$2.227 \times 10^{-5} \pm 4.93\%$	260	2421	1.839	12.11
500	$2.080 \times 10^{-5} \pm 7.72\%$	45	1412	1.849	11.25
1000	$1.742 \times 10^{-5} \pm 10.9\%$	22.5	1122	1.64	10.65

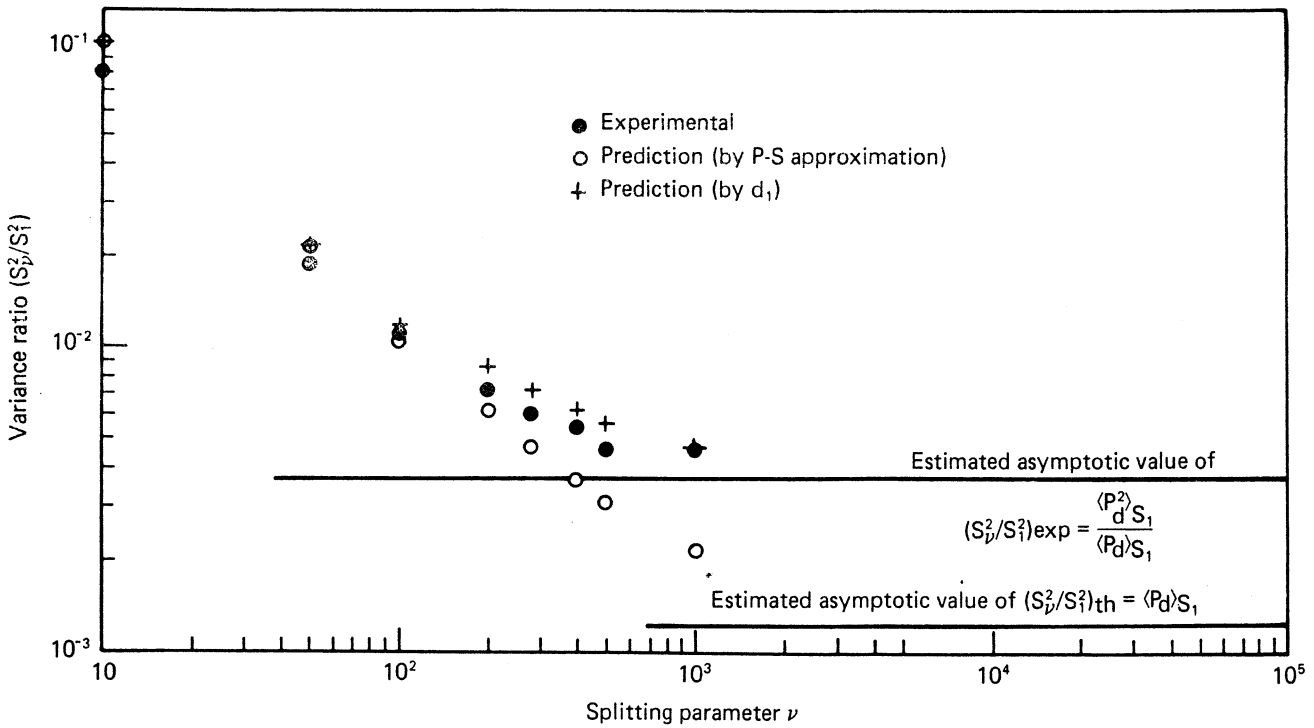


Fig. 3. Variance ratio versus splitting parameter.

example, for $\nu = 10$, using 20 000 source histories (5.2% of the sample of Table II) we obtain $P_d = 7.8 \times 10^{-4}$, $P_1 = 1.93 \times 10^{-2}$, and $\beta_1 = 0.69$, yielding $\nu_{opt} = 307$. Likewise, for 2000 source histories and $\nu = 1000$, we obtain $P_d = 1.412 \times 10^{-3}$, $P_1 = 1.36 \times 10^{-2}$, and $\beta_1 = 0.68$, yielding $\nu_{opt} = 275$. In general, at small values of ν, the advantage $(1/B)$ increases sharply [that is, $B(\nu)$ decreases] because of the $1/\nu$ behavior of $r_1(\nu)$ [Eqs. (67) and (68)]. In the optimum range, the variation of $B(\nu)$ is small because it is balanced by the still-decreasing variance ratio and linearly increasing time ratio, until the variance ratio reaches the neighborhood of its asymptotic value, where $B(\nu)$ will increase linearly. This behavior is expected to be typical of one-surface cases but is not expected to extend to the general case. Strong nonlinear behavior may increase the gradients and reduce the near-optimum range as n increases.

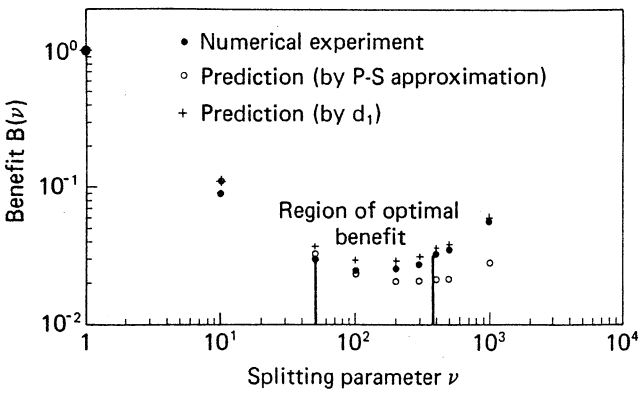


Fig. 4. Benefit $(B - q_\nu/q1)$ versus splitting parameter.

The above example suggests the following optimization algorithm. Calculation begins with any chosen value of ν, for instance, $\nu = 10$, and is carried on for 20 000 histories. (The size of this batch should be chosen for reasonable accuracy of bulk parameters.) This takes about 90 of the 2500 s required to get below 5% PRSD values at near optimum. The error in D is then still ≅50%. Then ν_{opt} is estimated (a very short run of 1000 analog histories will suffice to estimate β), yielding $\nu_{opt} = 307$, a near-optimum value. Accordingly, ν is changed and another batch at $\nu = 307$ is used to obtain ν_{opt}, based on an estimate of d_1. This process may be repeated using every history in the estimation of D. After 3.7% of the time required for an optimal 5% error calculation, we achieve satisfactory optimization improvement by a factor of ≅32 relative to analog Monte Carlo and 7% away from optimum (factor 35).

V.B. Problem 2

In problem 2, a similar homogeneous cylinder with the same energy groups and cross sections and an isotropic line source along the symmetry axis of the cylinder is considered. The detector is the total

leakage current through the circular envelope of the cylinder. The 100-cm-long cylinder has a r_{det} = 5-cm radius. The splitting surface is the cylindrical surface at r_{sp} = 2.5 cm. In this case, $D = 1.988 \times 10^{-2} \pm 0.97\%$, much larger than in the previous case. This difference will result in much smaller advantage of splitting, because P_1 and P_d are much larger (0.1306 and 0.1522, respectively). Thereby, we reach higher accuracy in comparing the variance ratio and the benefit, shown as a function of ν in Figs. 5 and 6. Both curves obtained from the P-S approximation underestimate the variance ratio and the benefit function. The P-S line is asymptotically parallel to the two other lines on a log-log scale. The estimation of ν_{opt} by the P-S approximation yields very satisfactory results ($6 \leqslant \nu_{opt} \leqslant 9$), which are well within the optimum range. All other features of small sample optimization were very similar to those of problem 1; at 3 to 5% of the total time, satisfactory values of ν_{opt} can be obtained for any starting $3 \leqslant \nu \leqslant 500$.

V.C. Problem 3

Problem 3 involves the cylindrical geometry of the first example, with normal plane source at x = 0 and total leakage detector at x_{det} = 10 cm. We now introduce two different media and apply survival biasing to the calculation. Material "a" extends from x = 0 to x = 5 cm and material b from x = 5 cm to x = 10 cm. The splitting surface is located at x = 6 cm within medium "b." Cross-section properties of both materials are given in Tables III and IV. Four energy groups are assumed for each material.

To demonstrate convergence, we chose a very large starting value of ν = 2000, and accumulated

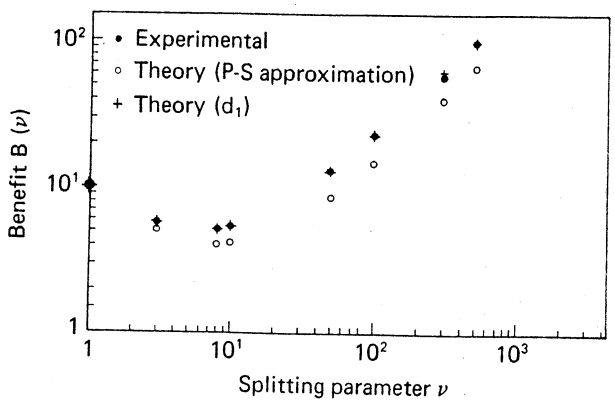


Fig. 6. Benefit ($B - q_\nu/q1$) versus splitting parameter.

information until the PRSD of D was ~50% ($D = 3.21 \times 10^{-2} \pm 50\%$). Then we computed the following quantities: P_1 = 0.104, P_d = 0.0587, $\langle w_1 \rangle$ = 0.5188, $\langle w_1^2 \rangle$ = 0.5004, $\langle w_d \rangle$ = 0.4979, and $\langle w_d^2 \rangle$ = 0.4427. An estimate of 0.5 was made for β. Using Eqs. (18) and (19), we obtained ν_{opt} = 23.15, which required 282 s. Then ν was changed to 23 and the run continued for another 252 s. The above quantities were computed, and this time β could be estimated from the two different batches, yielding β = 0.583. Again, ν_{opt} was estimated from the P-S approximation yielding ν_{opt} = 16.6. Using the ratio $(S^2_{2000}/S^2_{23})_{exp}$, d_1 was estimated to be 0.1315, resulting in ν_{opt} = 12. Figures 7 and 8 show the experimental variance ratio and benefit as functions of ν, derived from the large sample runs. The PRSD in these runs was ~3%, except for the last three points (500, 1000, and 2000), for which 10% was achieved. The theoretical values clearly follow the experimental results. Both

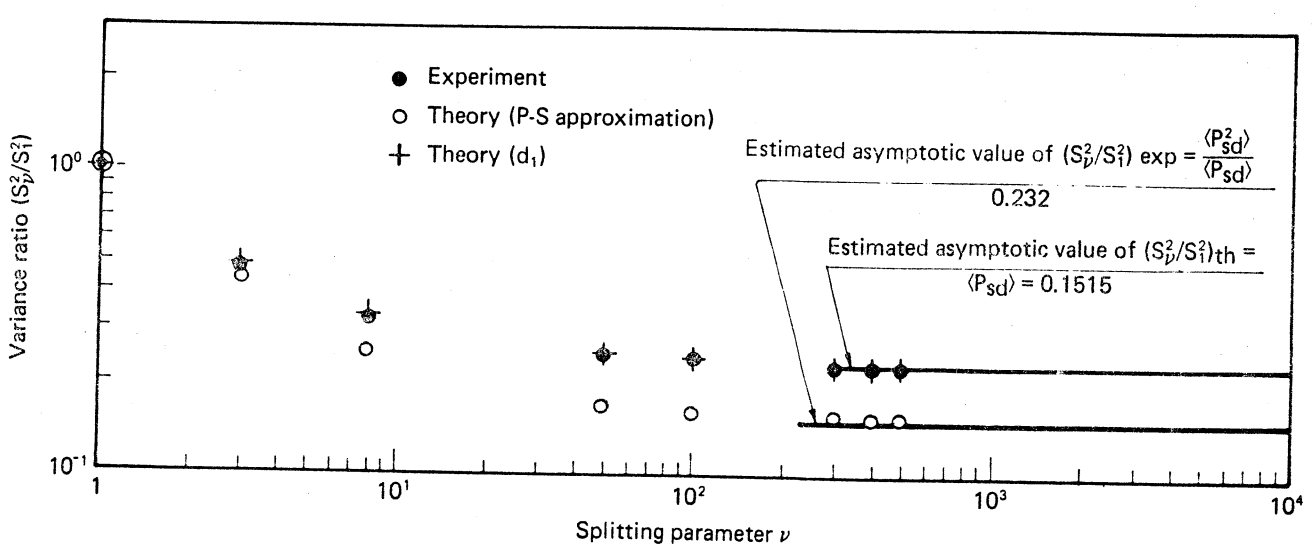


Fig. 5. Variance ratio versus splitting parameter.

TABLE III

Cross-Section Properties of Material A

Group	Σ_t (cm^{-1})	Σ_s/Σ_t	Into Group			
			1	2	3	4
1	0.4	1.0	0.25	0.25	0.25	0.25
2	0.6	0.67	0	0.25	0.25	0.25
3	0.8	0.5	0	0	0.25	0.75
4	1.0	0.4	0	0	0	1

TABLE IV

Cross-Section Properties of Material B

Group	Σ_t (cm^{-1})	Σ_s/Σ_t	Into Group			
			1	2	3	4
1	0.6	1.0	0.10	0.17	0.23	0.5
2	0.8	0.75	0	0.17	0.33	0.5
3	1.0	0.6	0	0	0.33	0.67
4	1.2	0.5	0	0	0	1

ν = 12 and ν = 17 are well within a satisfactory optimal range. At the optimal ν = 15, 2319 s was required to achieve 3%, a total of 534 s was used to obtain a near-optimum splitting value. However, after 282 s, we already had a reasonable value of ν = 23. The starting point of 2000 was deliberately exaggerated. Also, the PRSD limit of 50% could probably be lifted so that a smaller batch could be used. Batch size should depend on the error in the bulk parameters and not on D. Still, in general, the batch size required to obtain optimization is an essential topic for future studies.

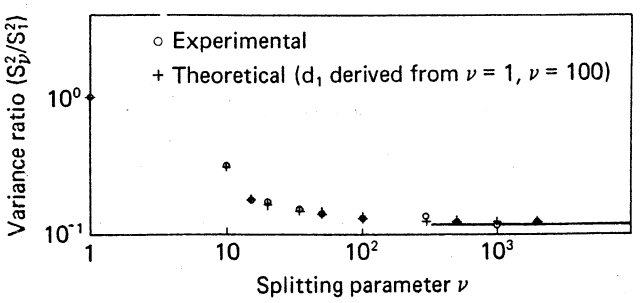


Fig. 7. Variance ratio versus splitting parameter.

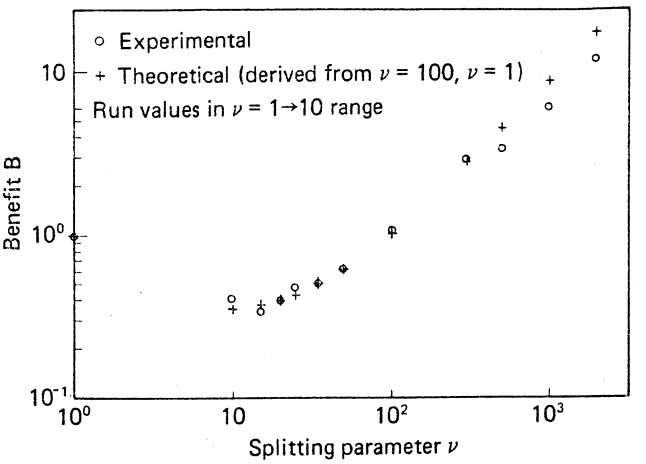


Fig. 8. Benefit versus splitting parameter.

V.D. Problem 4

The fourth problem involves two-dimensional geometry with two splitting surfaces (Fig. 9). An isotropic point source emits particles into the upper semicircle, which has a 3-cm radius; the detector is the integrated flux in the region enclosed by the S_d line and the circle circumference. Three energy groups are considered with cross-section properties shown in Table V.

The integrated flux is considered only over the upper two groups. Although analog Monte Carlo is used, $w_d \neq 1$ because the detector is not a leakage detector. A collision estimator is used for the flux, scoring $1/\Sigma_t$ at each collision point within the detector surface. Figure 10 displays very good agreement between the experimental values and the theoretical values of the variance ratio and benefit as a function of the splitting parameter. Here, ν was considered equal on both surfaces. The theoretical values of d_1 = 0.1035 and d_2 = 0.2105 were obtained by using three calculations of $r_2(2)$ and $r_2(8)$. Similar results were obtained for other pairs of values [for

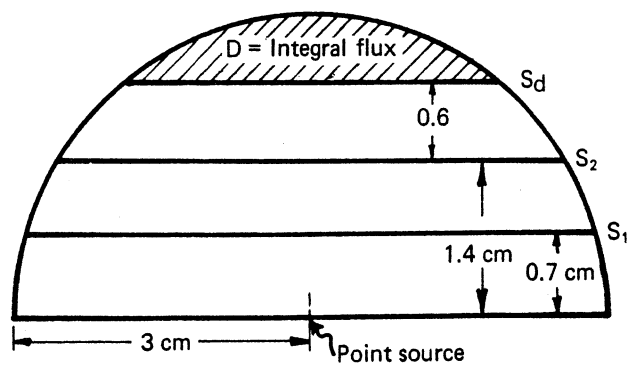


Fig. 9. Two-surfaces splitting geometry.

TABLE V

Cross Sections of Materials of Problem 4

Group	Σ_t (cm^{-1})	Σ_s/Σ_t	Into Group		
			1	2	3
1	1.0	0.9	0.7	0.9	0.0
2	2.0	0.75	0	0.5	0.5
3	1.0	1.0	---	---	1.0

example, from $r_2(6)$ and $r_2(25)$, we derive $d_1 = 0.1057$ and $d_2 = 0.2449$]. The P-S approximation also yields good results. For example, from $\nu = 8$, we obtain $P_2 = 0.04403$, $P_1 = 0.3210$, $P_d = 0.5191$, $\langle w_d \rangle = 0.9889$, and $\langle w_d^2 \rangle = 1.4529$, yielding

$$d_1 = \frac{P_2 P_d \langle w_d \rangle^2}{\langle w_d^2 \rangle} = 0.097$$

and

$$d_2 = \frac{P_d \langle w_d \rangle^2}{\langle w_d^2 \rangle} = 0.2223 \ .$$

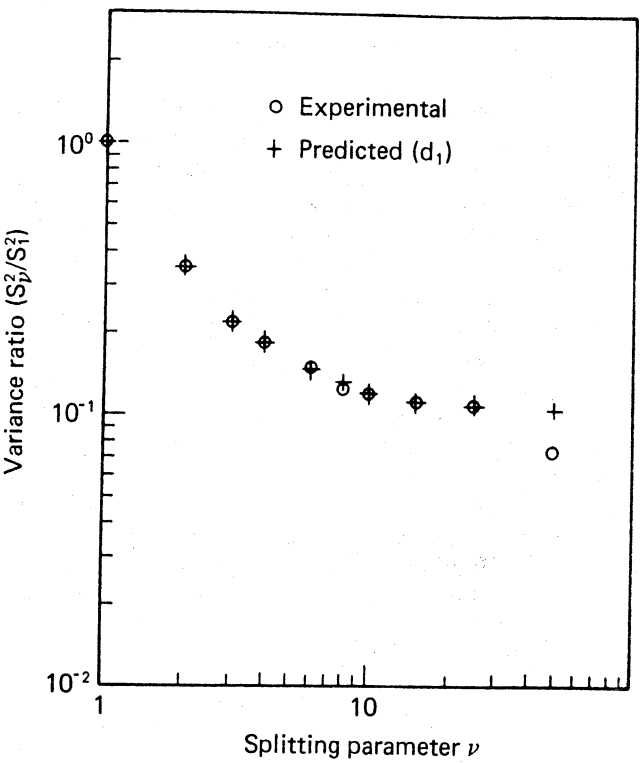
Obtaining the integrated flux $D = 5.816 \times 10^{-2} \pm 2.7\%$ required 30 s at the optimum $\nu = 3$. In this case, near-optimum, which is $2 \leqslant \nu_{opt} \leqslant 5$, was achieved after 6 s of calculation, using the P-S approximation and three small batches for the estimation of β_1 and β_2 (1.01 and 0.6453).

The above numerical results are in no way intended as a demonstration of the ultimate practicality of the method and the algorithms, but rather as a simple preliminary numerical test.

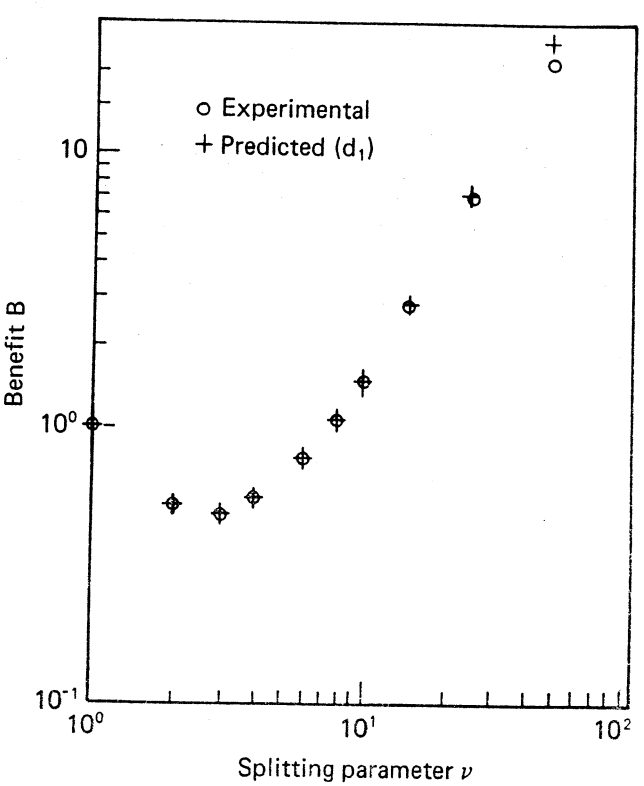
VI. CONCLUSIONS

A statistical model was presented by which a direct statistical approach yielded an analytic expression for the second moment, the variance ratio, and the benefit function in a model of an n surface-splitting Monte Carlo game.

In addition to the insight into the dependence of the second moment on the splitting parameters, the main importance of the expressions developed lies in their potential to become a basis for in-code optimization of splitting through a general algorithm. An approach to such an algorithm was briefly considered, consisting of a short run with some estimated splitting parameters. From this run, the bulk parameters can be derived and a first estimate of the optimum parameters can be reached using the P-S approximation and an estimated β. Then n more batches follow, after each of which ν_{opt} may be



(a)



(b)

Fig. 10. (a) Variance ratio and (b) benefit versus splitting parameter.

updated and used for the next run. After $n + 1$ batches, the d_i's and g_i's can be estimated and used for the final estimate of ν_{opt}.

Many questions remain for further investigation and generalization. It is essential to reach a near-optimum value for any in-code algorithm long before a target error is obtained for the selected response. Such a property seems difficult to prove generally, and the algorithm must be tested on a large spectrum of problems using some general multipurpose code before any final conclusions are drawn.

The knowledge of the d_i's and g_i's [specifically $B_n(\nu)$] may not be enough because if one assumes no limitation on the ν_i's, a problem of finding the minimum of a multivariable function arises. Assuming that all the ν_i's are equal will reduce the problem, but may yield only a local optimum. This general question deserves further consideration in an attempt to further illuminate the general properties of the benefit function. Furthermore, optimization can be considered with respect to the location and number of the splitting surfaces. This is a more difficult question in this model because the benefit is not an explicit function of these parameters. As mentioned earlier, an important extension of this model occurs when particles reach the detector by different routes and by crossing different splitting surfaces. Weight-dependent biasing methods as well as the possibility of $(n,2n)$ and fission should be studied.

ACKNOWLEDGMENTS

This work is dedicated to the memory of James L. Macdonald, an outstanding practitioner of the Monte Carlo method, who tragically did not live to see how right he was on some basic points. Lengthy discussions and debates with him motivated this work.

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