JOURNAL OF COMPUTATIONAL PHYSICS 32, 345–376 (1979)

Variance Reduction in Monte Carlo Computations using Multi-Dimensional Hermite Polynomials

F. H. MALTZ* AND D. L. HITZL

Lockheed Palo Alto Research Laboratory, 3251 Hanover St., Palo Alto, California 94304

Received September 6, 1978; revised October 27, 1978

This paper describes a new and promising technique for variance reduction in Monte Carlo computer simulations. This method, originally devised by Chorin in 1971, utilizes orthonormal Hermite polynomials as basis functions to form an approximation to the desired estimate. By properly applying this approach, estimates of much higher precision can be obtained so that the resulting Monte Carlo simulation exhibits an acceleration towards *convergence* which, furthermore, can be *controlled* by initial choices of certain adjustable parameters. The theory is thoroughly developed from first principles and simulation results are presented for both five- and twelve-variable model problems.

INTRODUCTION

Monte Carlo computations are frequently employed to obtain approximate values for statistical quantities such as the mean and variance of a desired (output) distribution. This approach is used since, in all but the simplest cases, the necessary integrals cannot be evaluated in closed form while, for problems with even a moderate number of input random variables ($\sim$3 to 5 say), direct numerical evaluation of the multi-dimensional integrals can be awkward and time consuming. Thus, one adopts a Monte Carlo approach in order to provide a *statistically realistic simulation* and accepts, however, the inherent shortcoming of results with rather low precision (i.e., limited accuracy).

The point of view taken in this paper is to regard Monte Carlo computations as a form of numerical quadrature [1, 2] with the only difference between Monte Carlo integration and conventional numerical integration being the method of dividing up the region of integration. With standard numerical integration packages, this division is usually performed in a regular fashion after, possibly, some initial transformation of variables. With Monte Carlo computations, however, an element of chance is included since sample values are determined using a pseudo random number generator [1, 3]. But, with the introduction of random number generators having special regularity properties [4], even the "chance mechanism" can be made less important.

A new and promising technique to reduce the error variance of Monte Carlo simulations is described in this paper. This method of *variance reduction* (or,

* Present Address: Naval Underwater Systems Center, New London, Connecticut 06320.

0021-9991/79/090345-32$02.00/0

equivalently, *convergence acceleration*) incorporates orthonormal function space expansions [3] in a procedure originally edveloped by Chorin [5] for evaluating one-dimensional problems in mathematical statistics. Recently, the Chorin method has been extended to multi-dimensional problems and several refinements to the basic Chorin procedure have been devised which can further reduce the Monte Carlo simulation errors for a wide class of linear and nonlinear problems (see also [6]). These refinements include:

(i) Using equal probability increment (so-called regulated) random numbers for low dimensional problems and their counterpart, equidistributed random numbers [4], in higher dimensions. In fact, this refinement has both theoretical justification [7] and practical importance; the latter has indeed been confirmed in all our Monte Carlo computer experiments.

(ii) Partitioning the set of samples—the so-called sample space—into subsets of equal or unequal size, forming various initial Chorin estimates, and obtaining a final composite estimate by averaging.

(iii) Optimizing the set of terms retained in an approximate series expansion using orthonormal polynomials. Presently, an adaptive series selection algorithm is being developed by the authors so that the computer can automatically perform this optimization for a wide class of problems.

As is known, it is possible to improve the ordinary Monte Carlo estimate by the use of certain approximating (smoothing) functions [3, 5]. In this paper, these basis functions are the multi-dimensional orthonormal Hermite polynomials [5, 8] which are used to form an approximation to the desired estimate. Previously, Hermite series expansions have been successfully applied to noise analysis problems [9] and to tracking filter simulation studies [10].

This paper is organized as follows. First, the basic Chorin estimator is developed from first principles and an expression for the Chorin error variance σ_C^2 is obtained. Then, using this formula, it is shown how the sampling scheme can be modified to further reduce this error variance. Next, the so-called symmetric (SC) and tri-symmetric (TSC) extensions of the Chorin estimator are discussed; it is shown that the TSC estimate yields a universally smaller Monte Carlo error variance than the basic Chorin estimate. After these theoretical developments, the technique we utilized to generate equidistributed random numbers is presented. Then, simulation results are described in detail for two model problems

1. The so-called Bullet Problem which represents a one-dimensional reentry trajectory having 5 random perturbation variables.

2. The so-called Deployment Dispersion Problem which models the dispersion of coasting trajectories after separation from a post-boost vehicle. This problem contains 12 random variables.

Next, a preliminary approach to an adaptive series selection algorithm is discussed and, finally, some practical considerations for computing with these advanced Monte Carlo estimators are outlined.

THEORETICAL BACKGROUND

In all Monte Carlo computations, the numerical error is a random variable. With the assumption of a "perfect" random number generator producing sample values at the input, the numerical error in the computations contains no bias and, after a large number (N) of individual trajectories, becomes asymptotically normally distributed. In ordinary (or direct) Monte Carlo, the error variance, as is well known, diminishes by the factor N^{-1}. The purpose then of variance reduction is to find Monte Carlo estimates which further reduce this error. These accelerated estimates consequently have higher precision than ordinary Monte Carlo estimates using the same number of sample trajectories.

Since all Monte Carlo computations can be regarded as an approximate form of numerical quadrature, this suggests that it should be possible to find estimates (for example, of the mean of a random function) which are better than those given by ordinary Monte Carlo procedures.

Presently, many methods are known for reducing the error variance in Monte Carlo computations. The class of methods described here is of the control variate type. The basic control variate method of variance reduction proceeds as follows. The ordinary Monte Carlo estimate

$$\hat{f} = \frac{1}{N}(f_1 + \cdots + f_N) = \frac{1}{N}\sum_1^N f_i \tag{1}$$

where $f_i = f(\mathbf{x}_i)$ for statistically independent samples

$$\mathbf{x}_i = \begin{bmatrix} x_i(1) \\ \vdots \\ x_i(p) \end{bmatrix}$$

is replaced by the control variate estimate

$$\bar{f} = E[g] + \frac{1}{N}\sum_1^N (f_i - g_i) \tag{2}$$

where the function g is chosen to approximate (or "mimic") the function f and, furthermore, to enable a closed form determination of $E[g]$. Whereas, in ordinary Monte Carlo, the computational error variance is

$$\sigma_{MC}^2 = \frac{\sigma^2}{N} \triangleq \sigma_D{}^2 \tag{3}$$

with $\sigma^2 \triangleq \mathrm{Var}[f] = E[f^2] - (E[f])^2$, the control variate estimate has numerical error variance

$$\sigma_{MC}^2 = \frac{\sigma_{CV}^2}{N} \tag{4}$$

with $\sigma_{CV}^2 = \mathrm{Var}[f - g]$. If the function g is chosen carefully, then it will turn out that $\sigma_{CV}^2 < \sigma^2$ giving variance reduction.

A problem with the control variate method is that it is usually not obvious, especially for high-dimensional problems, how to make a good choice for the mimic function g. The method we use, following Chorin [5], is to use a parametric family of functions

$$g = \sum_0^\infty a_i \Phi_i \tag{5}$$

where $\Phi_i = \Phi_i(\mathbf{x})$ belong to an orthonormal set, i.e., $E[\Phi_i \Phi_j] = \delta_{ij}$. In particular, we use the triangle family of polynomial functions where $\mathbf{x}$ is a gauss vector all of whose components have mean zero, variance one and are uncorrelated.

With this choice for the elements of $\mathbf{x}$, the Φ_i are then the orthonormal Hermite polynomials. For the single parameter case with $p = 1$

$$\begin{aligned}
\Phi_0 &= 1 \\
\Phi_1 &= x \\
\Phi_2 &= \frac{1}{(2)^{1/2}}(x^2 - 1) \\
\Phi_3 &= \frac{1}{(6)^{1/2}}(x^3 - 3x) \\
\Phi_4 &= \frac{1}{(24)^{1/2}}(x^4 - 6x^2 + 3) \\
&\vdots
\end{aligned}$$

For this case, the recursion formula

$$\Phi_{n+1}(x) = \frac{x}{(n+1)^{1/2}} \Phi_n(x) - \left(\frac{n}{n+1}\right)^{1/2} \Phi_{n-1}(x); \qquad n \geqslant 1 \tag{7}$$

is most useful.

In the multi-parameter case ($p > 1$), the general orthonormal Hermite polynomial is of the form $\Phi_{\iota_1}(x_1)\, \Phi_{\iota_2}(x_2) \cdots \Phi_{\iota_p}(x_p)$ with a restriction on the total order such that $\iota_1 + \iota_2 + \cdots + \iota_p \leqslant n$.

For finite second moment functions-that is, for integrable functions such that $E[|f|^2] < \infty$, the series given by Eq. (5) above converges in mean square, $\lim_{m\to\infty} E[|f - g_m|^2] = 0$, where $g_m = \sum_0^m a_i \Phi_i$ and $a_i = E[f\Phi_i]$. Therefore, the function $g \equiv f$ in this stochastic sense. The desired mean is a_0 since $\Phi_0 \equiv 1$. To use g_m for some $m \geqslant 1$ requires the evaluation of $a_1 \cdots a_m$. This is done by ordinary Monte Carlo using M additional samples $\mathbf{x}'$ as

$$\hat{a}_i' = \widehat{f\Phi_i'} = \widehat{f(\mathbf{x}')\, \Phi_i(\mathbf{x}')} \tag{8}$$

The mimic function now becomes

$$f_0 = \sum_0^m \hat{a}_i' \Phi_i \tag{9}$$

and the final estimator f^* (the basic Chorin estimator) is

$$f^* = \hat{f}' + \frac{1}{M} \sum_1^M (f_i - f_{0i}) \tag{10}$$

where

$$\hat{f}' = \frac{1}{M} \sum_1^M f(\mathbf{x}_i')$$

$$f_i = f(\mathbf{x}_i)$$

and

$$f_{0i} = \sum_0^m \hat{a}_k' \Phi_k(\mathbf{x}_i)$$

This estimate uses $N = 2M$ independent samples $(\mathbf{x}_1, \mathbf{x}_2, \ldots, \mathbf{x}_M)$ and $(\mathbf{x}_1', \mathbf{x}_2', \ldots, \mathbf{x}_M')$. Notice that this estimator is linear in f and can also be written in the form

$$\begin{aligned} f^* &= (\hat{f}' + \hat{f}) - \hat{f}_0 \\ &= 2D - I \end{aligned} \tag{11}$$

where D is the N-sample "direct (D) estimate"

$$D = \frac{1}{N} \left[\sum_1^M f(\mathbf{x}_i) + \sum_1^M f(\mathbf{x}_i') \right] \tag{12}$$

and I is the M-sample "indirect (I) estimate"

$$I = \frac{1}{M} \sum_1^M f_0(\mathbf{x}_i) \tag{13}$$

where $f_0(\mathbf{x}_i)$ is given by Eq. (9) above.

Chorin Estimator Statistics

The new estimate f^* is unbiased, that is

$$E[f^*] = E[f]$$

since (14)

$$E[\hat{f}] = E[f_0] = E[f].$$

The error variance is most conveniently obtained by first writing f^* in yet another form as follows

$$f^* = \hat{h} \triangleq \frac{1}{M} \sum_1^M h_i \tag{15}$$

where

$$h \triangleq f - \Delta f_0$$

and

$$\Delta f_0 \triangleq \sum_1^m \hat{a}_i' \Phi_i$$

Notice $f_0 = \hat{a}_0' + \Delta f_0$ so that Δf_0 is an estimate of the residual $f - E[f]$. In this form it is clear that f^* is a two step Monte Carlo since M-samples are drawn first to estimate the coefficients in the "corrector series" Δf_0 and then M additional samples are drawn to form the estimate $\hat{h}$. There will be a net variance reduction if the corrector series approximates Δf well in the stochastic sense defined earlier.

The corrector series is unbiased since $E[\Delta f_0] = 0$ and the error variance is

$$\begin{aligned} \sigma_C^2 &= \mathrm{Var}[f^*] \\ &= M^{-1}\{\sigma^2 + E[(\Delta f_0)^2] - 2E[f\,\Delta f_0]\} \end{aligned} \tag{16}$$

where, by orthogonality,

$$E[(\Delta f_0)^2] = \sum_1^m E[(\hat{a}_k')^2] \tag{17}$$

and, by projection,

$$E[f\,\Delta f_0] = \sum_1^m a_k E[\hat{a}_k'] \tag{18}$$

By definition,

$$E[(\hat{a}_k')^2] = M^{-1}\,\mathrm{Var}[f\Phi_k] + (E[f\Phi_k])^2$$

and, since $E[\hat{a}_k] = E[f\Phi_k] \triangleq a_k$, the exact Chorin variance is then

$$\sigma_C^2 = M^{-1}\left[R_m + M^{-1}\sum_1^m \sigma_k^2\right] \tag{19}$$

where, by orthogonality,

$$R_m = \sigma^2 - \sum_1^m a_k^2 = \sum_{m+1}^{\infty} a_k^2$$

and

$$\sigma_k^2 \triangleq \mathrm{Var}[f\Phi_k].$$

Here R_m is the mean square remainder in the m-truncated series expansion and will vanish as $m \to \infty$. Since the coefficients $a_k = E[f\Phi_k]$ are estimated, there is an added "penalty term" $M^{-2}\sum_1^m \sigma_k^2$ where σ_k^2 is the single sample error variance in the Monte Carlo estimate of a_k. Thus, the basic Chorin error variance has the general form

$$\sigma_C^2 = AM^{-1} + BM^{-2} \tag{20}$$

where the quantity $A \equiv R_m$ is monotonically non-increasing as $m \to \infty$ and B is monotonically non-decreasing as $m \to \infty$. Furthermore, $N = 2M$ sample trajectories are used in the complete Monte Carlo run.

Disproportionate Sampling

The basic Chorin estimator can be generalized to the extent that $N = 2M = M_1 + M_2$ where M_2 samples are to be used for corrector series coefficient estimates and M_1 samples are then used to determine the final estimate. By definition let $M = (N/2)$. For a fixed series truncation point m, there is an optimum allocation of samples (M_1, M_2) defined by k, $0 \leqslant k \leqslant M$ where

$$M_1 = M + k$$
$$M_2 = M - k.$$

The optimum value of k is chosen to minimize the Chorin variance

$$\begin{aligned}\sigma_C^2 &= AM_1^{-1} + B(M_1M_2)^{-1} \\ &= A(M + k)^{-1} + B(M^2 - k^2)^{-1}\end{aligned} \tag{21}$$

Since both A and B are non-negative, setting the derivative $d\sigma_C^2/dk = 0$ yields

$$(M - k)^2 = 2\left(\frac{B}{A}\right)k$$

for the unique optimal value of k. The ratio $R \triangleq (B/A)$ can be estimated by the same N samples as

$$\hat{R} = \frac{1}{N}\left[\sum_1^{M_1} \frac{B(\mathbf{x}_i)}{A(\mathbf{x}_i)} + \sum_1^{M_2} \frac{B(\mathbf{x}_i')}{A(\mathbf{x}_i')}\right] \tag{22}$$

Solving the above quadratic for the appropriate root and using $\hat{R}$ in place of R gives

$$\hat{k}_{\mathrm{opt}} = \hat{R} + M - (\hat{R}^2 + 2\hat{R}M)^{1/2} \tag{23}$$

SYMMETRIZATION

Disproportionate sampling depends upon how well the ratio R is estimated by $\hat{R}$. As an alternative to optimizing the allocation of samples, the Chorin estimator can be symmetrized in order to make better use of all the samples. For example, suppose two Chorin estimators are formed

$$\begin{aligned} f_1^* &= f^*(S, S') \\ f_2^* &= f^*(S', S) \end{aligned} \tag{24}$$

using the statistically independent sample sets

$$\begin{aligned} S &= \{\mathbf{x}_i\,,\ i = 1, 2,..., M\} \\ S' &= \{\mathbf{x}_i'\,,\ i = 1, 2,..., M\} \end{aligned}$$

Their average defines a "symmetrized Chorin estimate"

$$f_{SC}^* = \frac{f_1^* + f_2^*}{2} \tag{25}$$

This estimate has error variance

$$\sigma_{SC}^2 = \tfrac{1}{2}(\sigma_{C_1}^2 + \mathrm{Cov}[f_1^*, f_2^*]) \tag{26}$$

where $\sigma_{C_1}^2$ is the error variance for the estimate f_1^* (and f_2^* as well). The covariance term can be reduced to

$$\mathrm{Cov}[f_1^*, f_2^*] = E[\widehat{\Delta f_0}\ \widehat{\Delta f_0'}] \tag{27}$$

To show this, apply the definition

$$\mathrm{Cov}[f_1^*, f_2^*] = E[f_1^* f_2^*] - (E[f])^2, \tag{28}$$

use the form given by Eq. (15) for f_1^* and f_2^*, and expand $E[f_1^* f_2^*]$ in (28) as follows

$$E[f_1^* f_2^*] = E[\hat{f}\hat{f}'] - E[\hat{f}\ \widehat{\Delta f_2'}] - E[\hat{f}'\ \widehat{\Delta f_1}] + E[\widehat{\Delta f_1}\ \widehat{\Delta f_2'}]. \tag{29}$$

In (29) notice that

$$E[\hat{f}\hat{f}'] = E[\hat{f}]\,E[\hat{f}'] = (E[f])^2$$

and

$$E[\hat{f}\ \widehat{\Delta f_2'}] = E[\hat{f}'\ \widehat{\Delta f_1}] = \sum_1^m E[\hat{f}'\hat{a}_i'] \ E[\hat{\Phi}_i] = 0$$

since $E[\hat{\Phi}_i] = 0$. Therefore (29) becomes

$$E[f_1^* f_2^*] = (E[f])^2 + E[\widehat{\Delta f}_1 \, \widehat{\Delta f}'_2] \tag{30}$$

and substituting (30) into (28) gives the desired result (27).

Now use the definitions

$$\widehat{\Delta f}_0 = \sum_1^m \hat{a}_j \hat{\Phi}_j \, ; \qquad \widehat{\Delta f}'_0 = \sum_1^m \hat{a}_k \hat{\Phi}'_k \tag{31}$$

and substitute these into Eq. (27) to give

$$\mathrm{Cov}[f_1^*, f_2^*] = \sum_{j=1}^m \sum_{k=1}^m E[\hat{a}_k \hat{\Phi}_j] \, E[\hat{a}'_j \hat{\Phi}'_k] \tag{32}$$

It can readily be shown that

$$E[\hat{a}_k \hat{\Phi}_j] = \frac{1}{M} E[f \Phi_k \Phi_j]$$

$$E[\hat{a}'_j \hat{\Phi}'_k] = \frac{1}{M} E[f \Phi_j \Phi_k]$$

so that (32) becomes

$$\mathrm{Cov}[f_1^*, f_2^*] = M^{-2} \sum_{j=1}^m \sum_{k=1}^m (E[f \Phi_j \Phi_k])^2 \tag{33}$$

Then, substituting Eq. (33) into (26) gives the final result, the exact error variance for the symmetrized Chorin estimate

$$\sigma_{SC}^2 = \frac{1}{2} \left\{ \sigma_{C_1}^2 + M^{-2} \sum_{j=1}^m \sum_{k=1}^m (E[f \Phi_j \Phi_k])^2 \right\} \tag{34}$$

which, for large M, is

$$\sigma_{SC}^2 \cong \frac{1}{2} \sigma_{C_1}^2 \cong \frac{R_m}{N} \tag{35}$$

This further asymptotic variance reduction is obtained at the expense of the additional second order penalty term shown in (34).

We next show that it is possible to achieve the fully reduced asymptotic variance R_m/N together with a simultaneous reduction in the second order penalty term of the basic Chorin estimator. This is done by partitioning the sample space into three statistically independent sets S, S' and S'' of M samples each

$$S = \{\mathbf{x}_i \, , \, i = 1, 2, \ldots, M\}$$

$$S' = \{\mathbf{x}'_i \, , \, i = 1, 2, \ldots, M\}$$

$$S'' = \{\mathbf{x}''_i \, , \, i = 1, 2, \ldots, M\}$$

and forming the three estimates

$$\begin{aligned} f_1^* &= f^*(S, S') \\ f_2^* &= f^*(S', S'') \\ f_3^* &= f^*(S'', S) \end{aligned} \tag{36}$$

The average of these estimates then defines a "tri-symmetrized Chorin estimate,"

$$f_{TSC}^* = \frac{f_1^* + f_2^* + f_3^*}{3} \tag{37}$$

It is shown elsewhere [6] that the three estimates f_i^* are mutually uncorrelated so that there is no additional penalty term. In addition, since $N = 3M$, the error variance for this estimate is

$$\sigma_{TSC}^2 = \frac{\sigma_{C_1}^2}{3} \tag{38}$$

where $\sigma_{C_1}^2$ is the Chorin variance for any one of the above three estimates. The final result for the exact *TSC* error variance is

$$\sigma_{TSC}^2 = AN^{-1} + 3BN^{-2} \tag{39}$$

which should be compared with

$$\sigma_C{}^2 = 2AN^{-1} + 4BN^{-2} \tag{20}$$

for the basic Chorin estimator.

Notice that both first and second order terms are smaller for the error variance associated with this estimate f_{TSC}^*. Therefore, $\sigma_{TSC}^2 \leqslant \sigma_C{}^2$ for all A, B and N and the basic Chorin estimator is not optimal.

To summarize, the exact Monte Carlo error variance expressions are given below for the three estimators f^*, f_{SC}^* and f_{TSC}^*. Note that, in all cases, the leading term gives an asymptotic (first order) value for large $N \to \infty$.

$$\begin{aligned} \sigma_C{}^2 &= 2AN^{-1} + 4BN^{-2} \\ \sigma_{SC}^2 &= AN^{-1} + 2(B + C)\, N^{-2} \\ \sigma_{TSC}^2 &= AN^{-1} + 3BN^{-2} \end{aligned} \tag{40}$$

where

$$A = \sigma^2 - \sum_1^m a_k{}^2 \triangleq R_m = \sum_{m+1}^{\infty} a_k{}^2$$

$$B = \sum_{1}^{m} \sigma_k^2$$

$$C = \sum_{1}^{m} \sum_{1}^{m} b_{jk}^2$$

and

$$a_k \triangleq E[f\Phi_k]$$
$$\sigma_k^2 \triangleq \mathrm{Var}[f\Phi_k]$$
$$b_{jk} \triangleq E[f\Phi_j\Phi_k].$$

Overview

Based upon the previous theoretical developments, the general situation is illustrated schematically in Fig. 1 where the Monte Carlo error variance σ_{MC}^2 is sketched as a function of trajectory sample size N. Considering the estimand to be a polynomial of some degree n, the method of Ermakov and Zolotukhin [11, 12] can (theoretically) obtain exact correction and estimates with $\sigma_{MC}^2 = 0$ for $N \geqslant n$. Hence the curve labelled $E - Z$ is shown as a possible lower boundary of the allowable region for

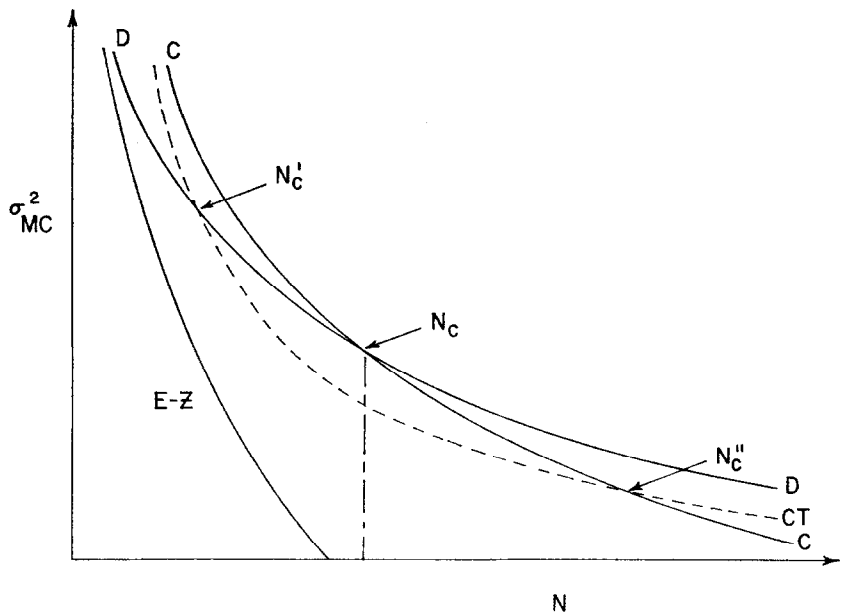

FIG. 1. Typical behavior for the Monte Carlo error variance σ_{MC}^2 as a function of the number of sample trajectories N. Here D = Direct, C = Chorin, CT = Truncated Chorin, and $E - Z$ = Ermakov and Zolotukhin estimates. Various cross-over points N_c, N_c' and N_c'' are also labelled.

variance reduction. The upper boundary is furnished by the direct estimate D. The desire, of course, is to simultaneously decrease both σ_{MC}^2 and N.

For small N, the Chorin estimator initially exhibits a variance penalty but, at some value of N depending upon the particular function and correction series with suitably large m, $\sigma_C{}^2 = \sigma_D{}^2$. This value of N is referred to as the fixed correction series "cross-over" point N_c. For all $N > N_c$, $\sigma_C{}^2 < \sigma_D{}^2$.

Further reduction in variance can be obtained by optimizing the selection of terms retained in the corrector series. By dropping terms below a certain threshold (which is itself a function of N), a so-called Truncated Chorin estimate CT will have two cross-over points N_c', N_c'' as shown. Thus, for low to moderate sample sizes, an advantage accrues if the approximate series expansion is simplified and shortened while, for large N, there is a variance penalty.

Equidistributed Random Numbers

In all Monte Carlo computer experiments, the sample values $\mathbf{x}_i$ determined by the "random number generator" should fill the p-dimensional parameter space in a uniform manner. For low dimensional problems ($p \leqslant 4$ say), sampling can be done in a completely regular fashion with n samples per parameter spaced at equal probability increments. A full factorial sampling plan is then completed in the computer simulation yielding $N = n^p$ individual trajectories. Since $n \geqslant 4$, the use of these so called "regulated random numbers" is perfectly feasible if p is small; in fact, excellent results have been obtained for $p = 4$. On the other hand, for larger values of p, a factorial sampling plan must be abandoned.

While still attempting to maintain, however, a uniform distribution of sample values in the parameter space, we were then led to consider so called equidistributed random numbers [4]. In our computations, the successive prime numbers $p_i = 2, 3, 5, 7, 11, 13, 17,\ldots$ were used and, for $1 \leqslant k \leqslant N$, the fractional part of $k(p_i)^{1/2}$ calculated. The values $n_i \triangleq \text{Frac}(k(p_i)^{1/2})$ so determined are then equidistributed in the unit interval ($0 < n_i < 1$) and, utilizing the well-known Box–Muller transformation [1]

$$\begin{aligned} x_i &= (-2 \ln n_i)^{1/2} \cos(2\pi n_{i+1}) \\ x_{i+1} &= (-2 \ln n_i)^{1/2} \sin(2\pi n_{i+1}), \end{aligned} \tag{41}$$

normalized random variables with zero mean and unit variance are generated.

For the two model problems to be described in the next section, the Monte Carlo experiments were performed using a variety of random number generators. In all cases, the most accurate and consistent results were obtained using the equidistributed random number generator described above.

However, a problem does remain. Plots were made of several thousand successive points for

(a) $\text{Frac}(k(3)^{1/2})$ vs $\text{Frac}(k(2)^{1/2})$

(b) Frac$(k(11)^{1/2})$ vs Frac$(k(7)^{1/2})$, and

(c) Frac$(k(13)^{1/2})$ vs Frac$(k(11)^{1/2})$.

For case (a), the points filled the unit rectangle very uniformly and evenly; for the other two cases, however, the points formed narrow bands and left large regions of the unit rectangle empty. Results for case (c) are shown in Fig. 2 for $1 \leqslant k \leqslant N$ with $N = 4000$. Examining this picture, it is easy to find the low-order resonance relation

$$6(13)^{1/2} - 2(11)^{1/2} - 15 = 5.807 \times 10^{-5} \triangleq \Delta$$

which shows that for $N > \Delta^{-1} \approx 17221$, the bands would merge and the unit rectangle would then be completely filled. For large N, however, new bands would reappear.

Thus, in order to achieve truly equidistributed sample points in a p-dimensional unit "cube" without undesirable clustering, both the prime numbers p_i and the total sample size N should be chosen with some care. These ideas are presently being investigated.

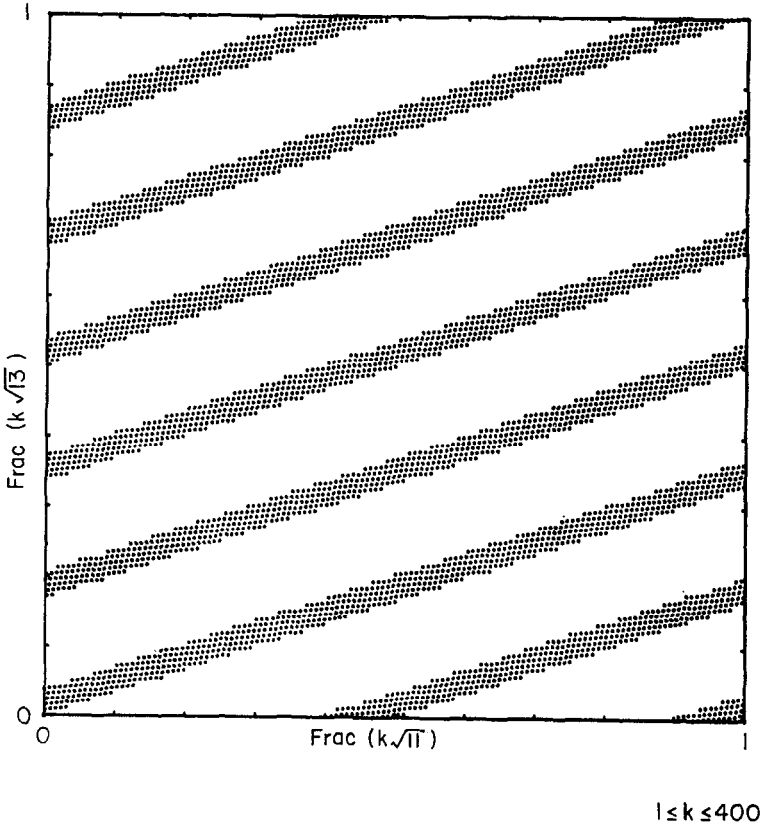

FIG. 2. Clustering of successive points using an "equidistributed" random number generator. A total of 4000 points are plotted.

Model Problems

Two model problems are treated in detail in this paper. The first is a simplified one-dimensional model for a ballistic reentry trajectory having random perturbations in the dynamics. This so-called "Bullet Problem" is defined by the differential equations

$$\begin{aligned} \dot{x} &= \alpha v + \beta \\ \dot{v} &= \gamma x + \delta v + \epsilon \end{aligned} \tag{42}$$

and the nominal ($\beta = \epsilon = 0$) initial conditions x_0 and v_0. Each of the 5 coefficients α, β, γ, δ, ϵ is non-time-varying but is assumed to have the form

$$\rho = \rho_0 + \rho'$$

with a nominal value ρ_0 and a random component ρ'. Setting

$$\zeta \triangleq (\delta^2 + 4\alpha\gamma)^{1/2} \tag{43}$$

and

$$r_1, r_2 = \tfrac{1}{2}[\delta \pm \zeta] = -\tau_1^{-1}, -\tau_2^{-1} \tag{44}$$

for the two "time constants" τ_i, the solution of (42) is

$$x(t) = C_1 e^{r_1 t} + C_2 e^{r_2 t} + \frac{\alpha\epsilon - \delta\beta}{2\alpha\gamma}\left[e^{r_1 t} + e^{r_2 t} - 2\right] \tag{45}$$

with

$$\begin{aligned} C_1 &\triangleq \frac{1}{2}\left(1 - \frac{\delta}{\zeta}\right) x_0 + \frac{\alpha}{\zeta} v_0 \\ C_2 &\triangleq \frac{1}{2}\left(1 + \frac{\delta}{\zeta}\right) x_0 - \frac{\alpha}{\zeta} v_0 \end{aligned} \tag{46}$$

where x_0 and $v_0 = (1/\alpha)\,\dot{x}(0)$ are the *nominal* initial conditions at $t = 0$ with both random noise terms β and ϵ equal to zero. Also, using (42),

$$v(t) = \frac{1}{\alpha}\left[\dot{x}(t) - \beta\right]$$

while $\dot{x}(t)$ is immediately computable from (45).

For the simulations, the following nominal values

$$\begin{aligned} \alpha_0 &= 1.0 \\ \beta_0 &= 0.0 \\ \gamma_0 &= -0.8 \\ \delta_0 &= -2.4 \\ \epsilon_0 &= 0.0 \end{aligned}$$

were chosen for the five parameters. The corresponding time constants are then $\tau_1 = 2.5$, $\tau_2 = 0.5$. Next, we wish to allow some variability in the parameter set $(\alpha, \beta, \gamma, \delta, \epsilon)$ while maintaining the inequalities

$$\begin{aligned} \alpha &> 0 \\ \delta &< 0 \\ -\delta^2/4\alpha &< \gamma < 0 \end{aligned} \tag{47}$$

so that the solution $x(t)$, $v(t)$ is indeed given by two decaying exponentials.

Using the equidistributed random number generator described previously, so called normal zero-one $N(0, 1)$ Gaussian random numbers ξ were produced with a theoretical

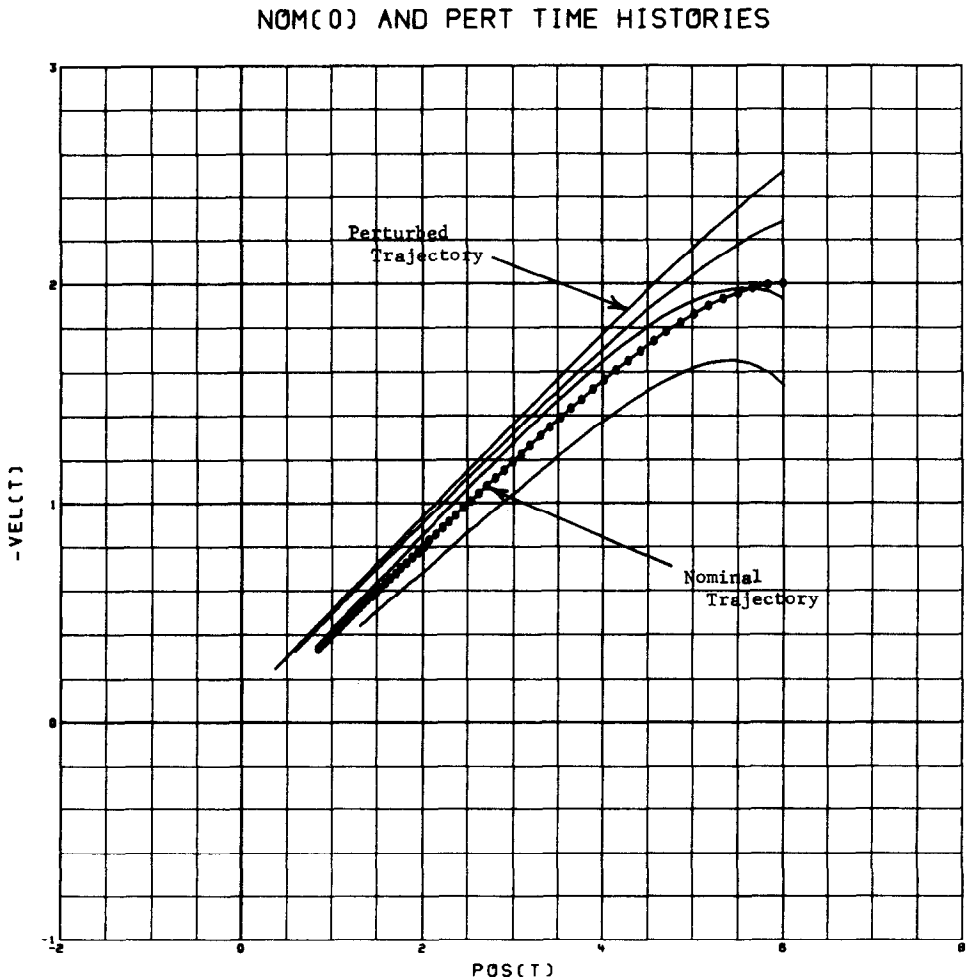

FIG. 3. The nominal and four perturbed trajectories for the "Bullet Problem."

mean of zero and variance of one. Hence, in order to maintain reasonably small perturbations about the nominal trajectory and to guarantee that $\zeta^2 > 0$ "almost always," the following scaling values s_ρ

$$s_\alpha = 0.05$$
$$s_\beta = 0.10$$
$$s_\gamma = 0.08$$
$$s_\delta = 0.07$$
$$s_\epsilon = 0.10$$

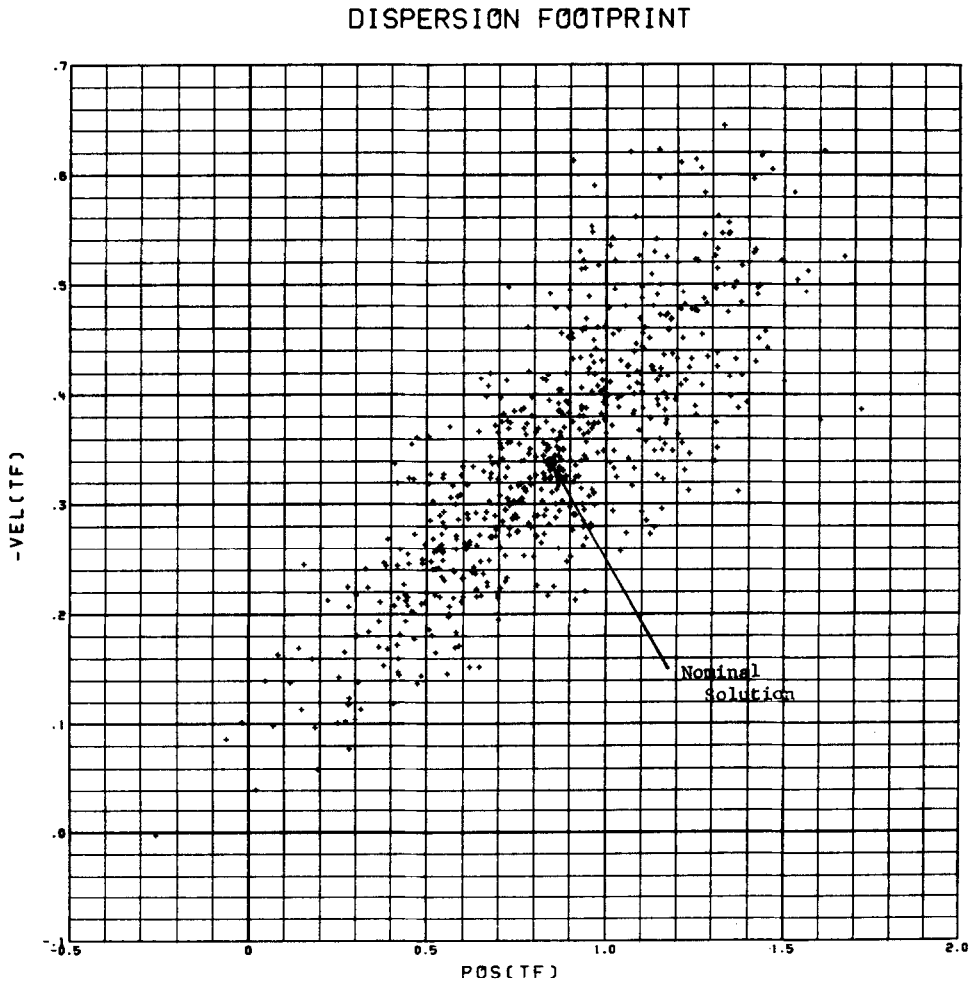

FIG. 4. The impact dispersion footprint for the "Bullet Problem"; a total of 600 impact points are plotted.

were introduced for each of the five parameters so the random components are then given by

$$\rho' = s_\rho \xi. \tag{48}$$

To illustrate, Fig. 3 shows the nominal and four perturbed trajectories for the following "standard" case

$$x_0 = 6.0 \qquad v_0 = -2.0 \qquad t_f = \text{final time} = 2\tau_1 = 5.0. \tag{49}$$

Note that, since the approach is always towards the origin, the vertical axis is $-v(t)$. Furthermore, several additional features are evident in Fig. 3 and can be understood

and $v(t) \to 0$ as $t \to \infty$ while the random perturbations—which have fixed values for any given trajectory—only affect

$$v(0) = v_0 - \frac{\beta}{\alpha} + \frac{\alpha\epsilon - \delta\beta}{2\alpha\gamma}\frac{\delta}{\alpha}$$

and not $x(0) = x_0$.

Continuing, a so-called impact dispersion footprint is shown in Fig. 4 for the standard case defined previously in Eq. (49). Impact points for the nominal and 600 perturbed trajectories are plotted here. Note that the final time t_f is different for each perturbed trajectory by virtue of Eqs. (43) and (44). The nominal impact point has the coordinates

$$x(t_f = 5) = 0.84583 \cdots$$
$$v(t_f = 5) = -0.33832 \cdots.$$

Now, in order to apply the basic Chorin estimator to this problem, both the series truncation point [m in Eq. (9)] and the appropriate parameters to include in $\mathbf{x}$ must be determined. The total number of terms

$$m = m(n, p) \tag{50}$$

in the p parameter Hermite polynomial expansion of the estimator is given in Table 1 for various values of n. The quantity n is the highest order polynomial to be retained in the generalized orthonormal series; $n = 0$ corresponds then to standard (or Direct) Monte Carlo with the single constant polynomial $\Phi_0 = 1$ independent of the number of parameters p. In particular, note how successive values are obtained by summing two neighboring quantities. For any n and p, a particularly elegant formula has been found

$$m = m(n, p) = \sum_{l=0}^{\min(n,p)} \binom{n}{l}\binom{p}{l} = \binom{n+p}{n} = \binom{n+p}{p} = \frac{(n+p)!}{n!\,p!} \tag{51}$$

where

$$\binom{n}{l} = \text{binomial coefficient} = \frac{n!}{l!\,(n-l)!}$$

TABLE 1

Maximum Number of Terms $m(n, p)$ in the p — Parameter Hermite Series Expansion

	n				
p	0 (constant)	1 (linear)	2 (quadratic)	3 (cubic)	4 (quartic)
1	1	2	3	4	5
2	1	3	6	10	15
3	1	4	10	20	35
4	1	5	15	35	70
5	1	6	21	56	126

To determine which of the 5 parameters to include in the Hermite expansion, numerical partial derivatives were computed about the nominal solution for the "standard" case specified in (49). Results are given in Table 2 below. Using this Table, the parameters were then ranked according to sensitivity and, after an extensive series of simulation runs to determine the parameter set maximizing variance reduction, the three quantities α, β and γ were chosen. Hence $p = 3$. Then computations were performed for various $n = 1, 2, \ldots$.

TABLE 2

Numerical Partial Derivatives

Parameter ρ	α	β	γ	δ	ϵ
$\partial x(t_f)/\partial\rho$	0.10552	2.79692	−0.34329	0.15839	1.16538
$\partial v(t_f)/\partial\rho$	−0.12649	−0.91866	0.66545	−0.27451	0.03388

Sample results from these calculations are shown in Figs. 5 to 8 for the mean position and velocity at t_f produced using both the Direct estimator given in (12) and the basic Chorin estimator specified by (10) or (11). Also, for comparison, the

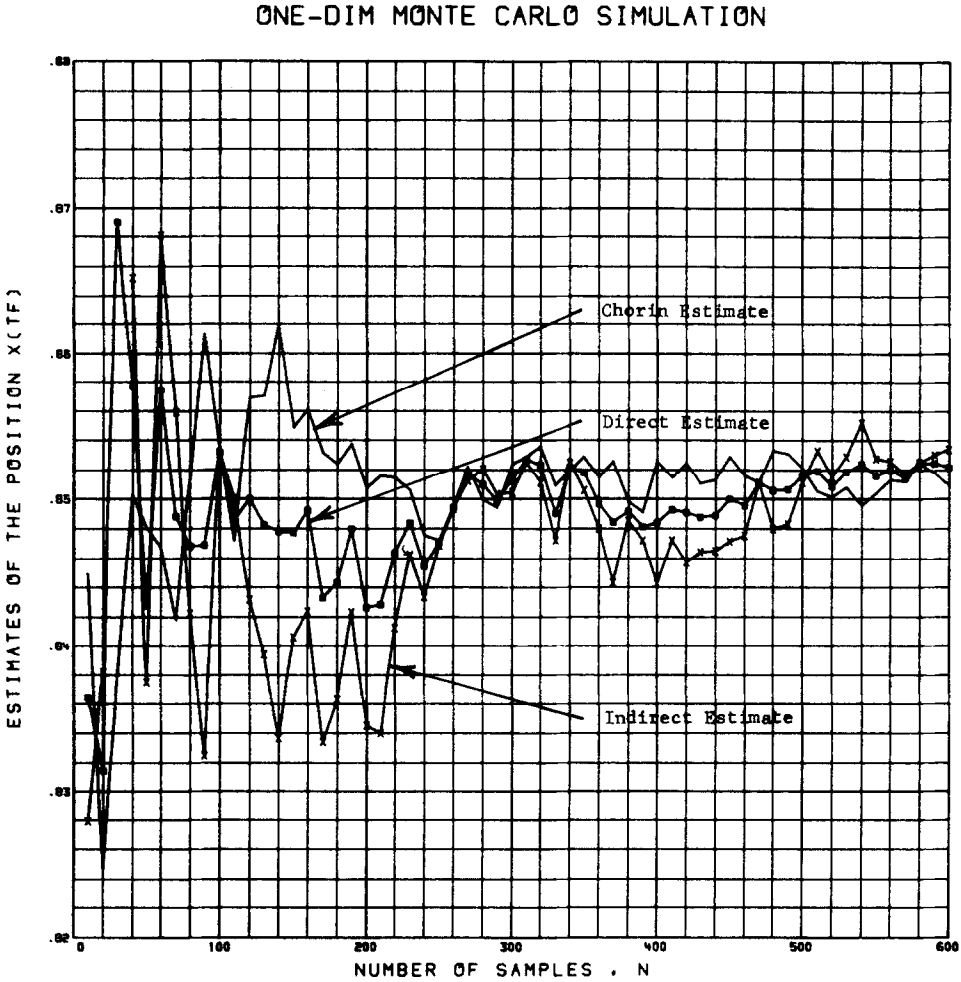

FIG. 5. Three estimates for the position at the final time $x(t_f)$. The converged final value is $x(t_f) = 0.851\ldots$.

Indirect Chorin estimate given by (13) is shown. Here $n = 1$ so $m(1, 3) = 4$. Note the convergence of all three estimators as N, the total number of sample trajectories, is increased.

The payoff is shown in Figs. 6 and 8 where the Monte Carlo error variance for the position and velocity estimates is plotted as a function of trajectory sample size N. Even for small values of $N < 60$, the Chorin variance is far below the corresponding Direct variance and, moreover, this behavior is maintained continuously as N is increased.

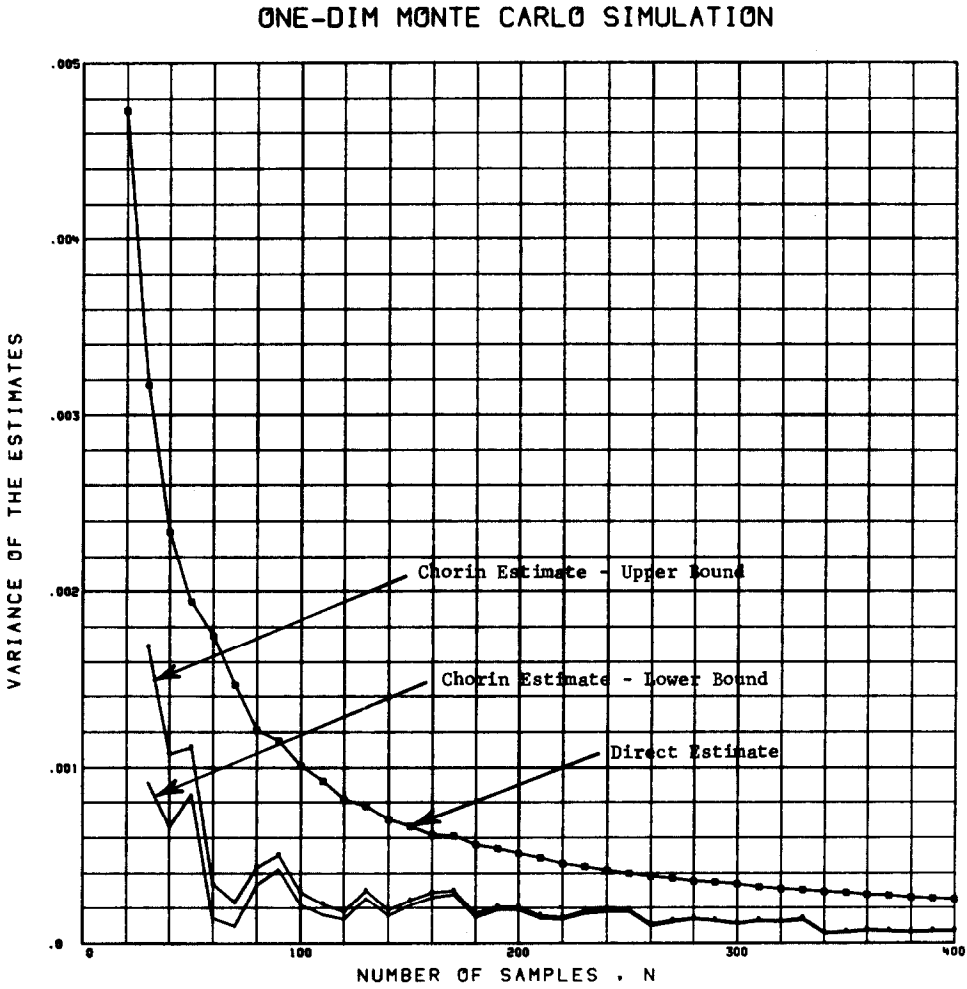

FIG. 6. Monte Carlo error variances for the Direct and Chorin estimates. The exact value for the Chorin variance σ_C^2 lies between the two bounding curves.

Returning to Eq. (19), the Chorin variance is given by

$$\sigma_C^2 = \left(\sigma^2 - \sum_1^4 a_k^2\right) M^{-1} + \left(\sum_1^4 \mathrm{Var}[f\Phi_k]\right) M^{-2} \tag{52}$$

with f either $x(t_f)$ or $v(t_f)$. The lower bound shown in Figs. 6 and 8 is computed by simply neglecting the second order term. The upper bound is obtained by noting

$$\mathrm{Var}[f\Phi_k] \triangleq E[(f\Phi_k)^2] - (E[f\Phi_k])^2 \leqslant E[f^2\Phi_k^2]. \tag{53}$$

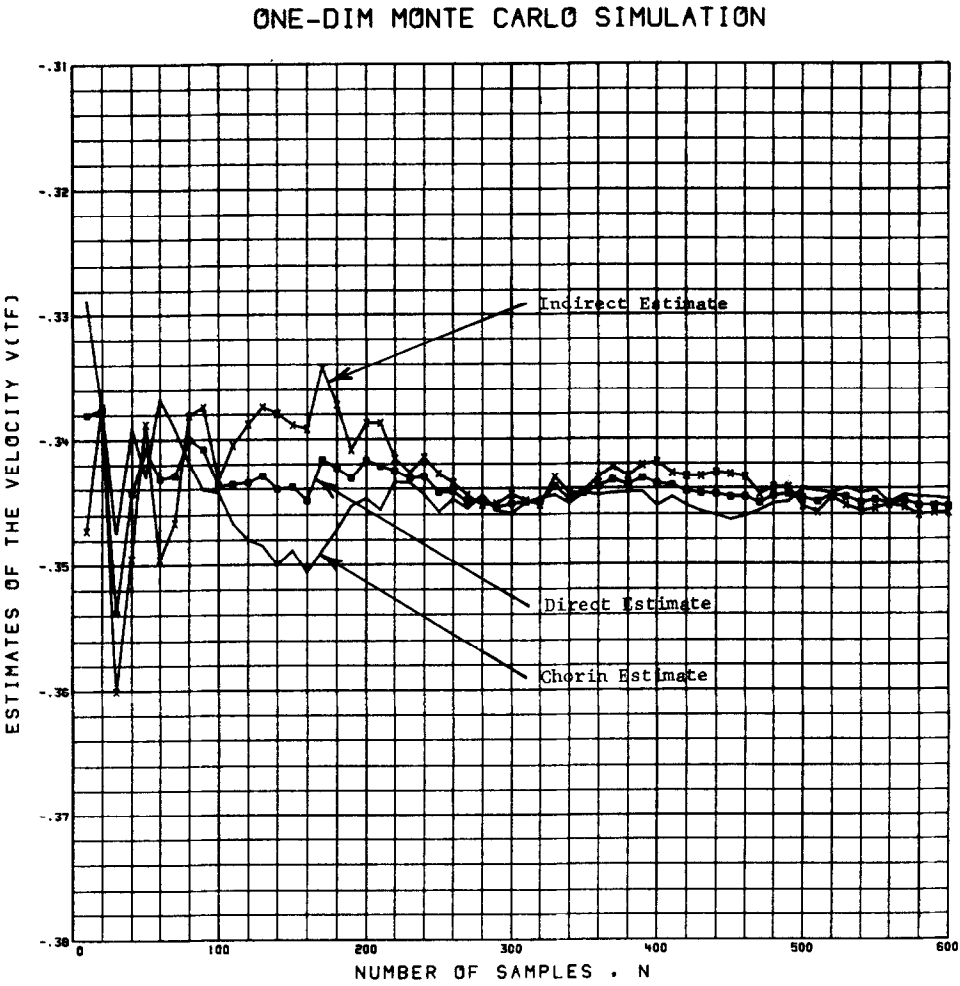

FIG. 7. Three estimates for the velocity at the final time $v(t_f)$. The converged final value is $v(t_f) = -0.345\ldots$.

The second model problem is considered now. This so called Deployment Dispersion Problem is defined by the 12 parameter function

$$\mathbf{y} = \boldsymbol{\mu} + A\mathbf{x} + \tfrac{1}{2}(\mathbf{x}^T B\mathbf{x})\mathbf{c} \tag{54}$$

where

$$\mathbf{y} = \begin{bmatrix} y_1 \\ y_2 \\ y_3 \end{bmatrix} \text{ is a three vector of resultant trajectory dispersions}$$

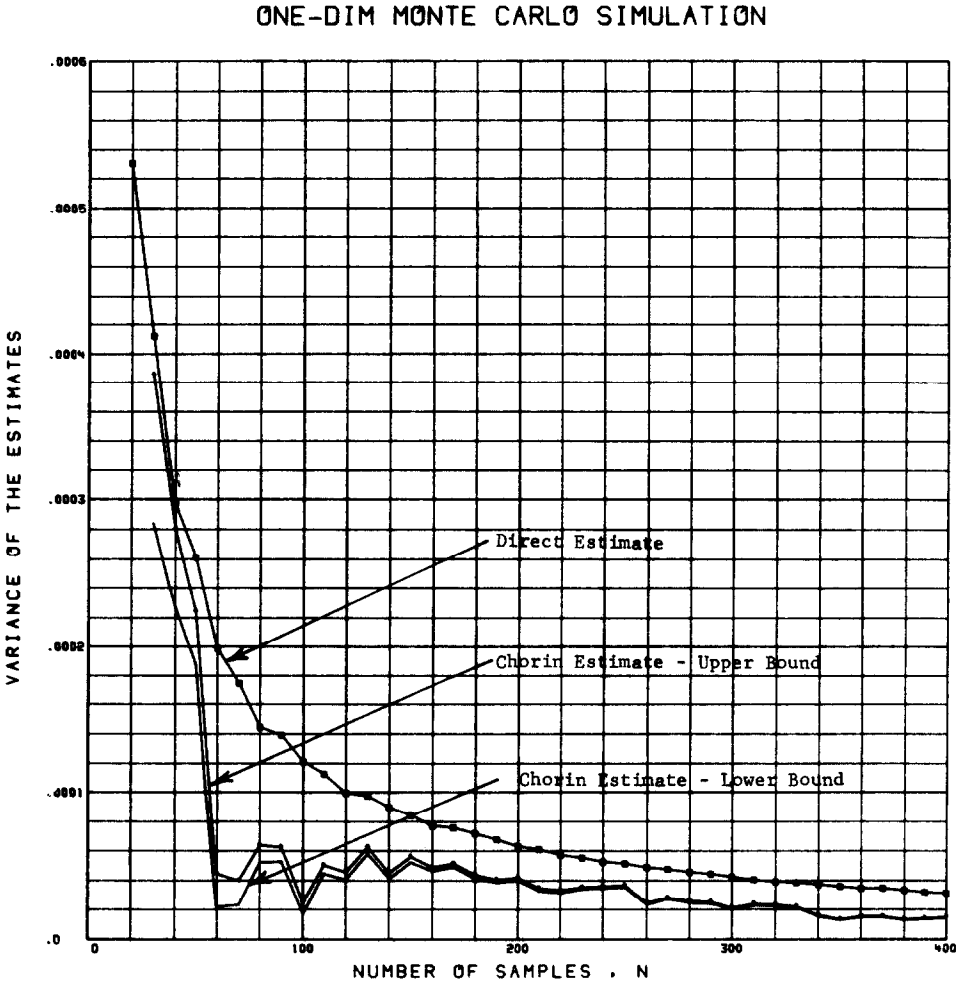

FIG. 8. Monte Carlo error variances for the Direct and Chorin estimates. Note the ten-fold reduction in velocity error variance compared to the position error variance shown in Fig. 6.

$\mathbf{x}^T = [x_1, x_2, \ldots, x_{12}]$ is a twelve vector of input random errors resulting from four basic error sources

A is a (3×12) matrix with constant entries

B is a (12×12) matrix with constant entries

and

μ, $\mathbf{c}$ are three vectors with constant entries.

This function was devised to simulate the effect of multiple error sources $\mathbf{x}$ on the

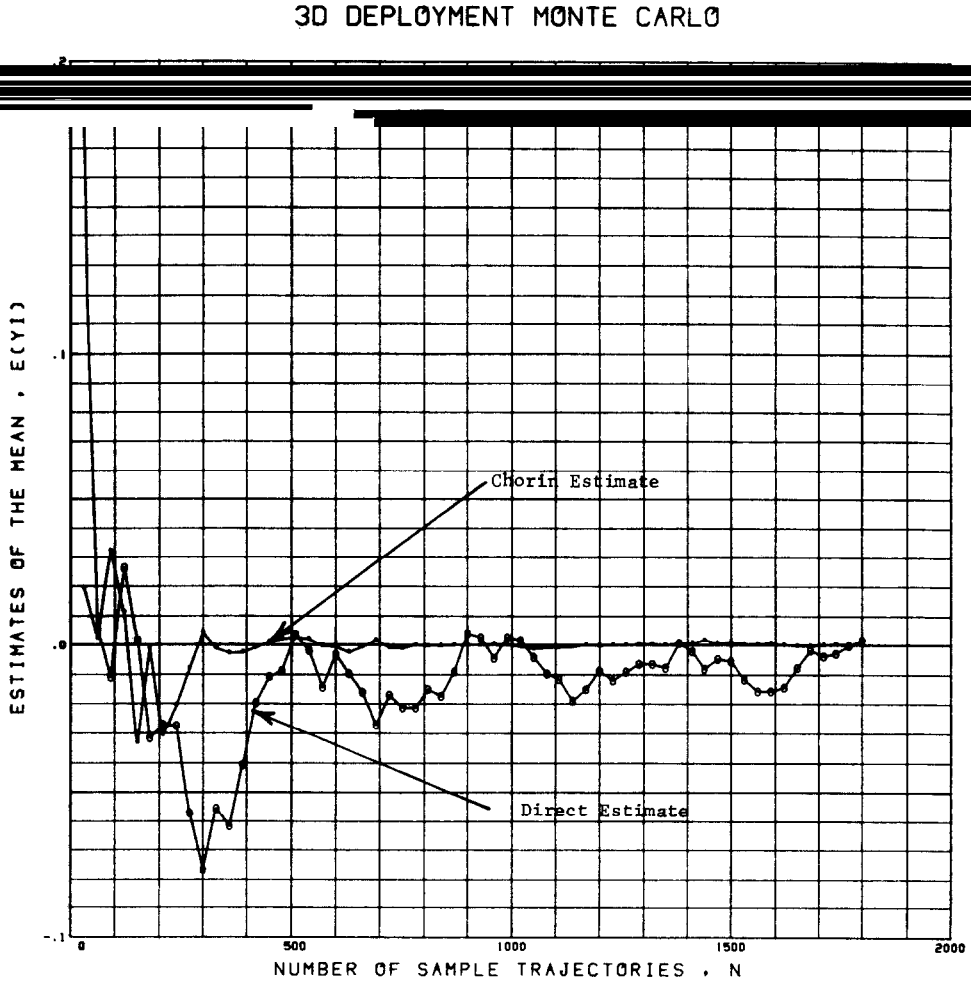

FIG. 9. Direct (○) and Chorin (*) estimates of the quantity y_1 for the deployment dispersion function $\mathbf{y} = A\mathbf{x} + \mu$ with $E[y_1] = 0$. This linear problem has 5 terms in the correction series.

resultant dispersion **y** of coasting trajectories in three dimensions after deployment from a post boost vehicle. For the Monte Carlo experiments, the principal purposes of this model were

- To test numerically the dimension limitation when no initial transformation of input variables is performed.
- To furnish a simple analytic structure so the Hermite polynomial expansion can be tailored exactly.

For the results shown in Figs. 9 to 11, the A and B matrices were chosen with all integer entries as follows

$$A = \begin{bmatrix} 1 & 0 & 0 & 1 & 0 & 0 & 1 & 0 & 0 & 1 & 0 & 0 \\ 1 & 3 & 2 & 0 & 3 & 2 & 1 & 3 & 0 & 0 & 3 & 0 \\ 1 & 2 & 3 & 0 & 1 & 3 & 2 & 0 & 3 & 2 & 1 & 3 \end{bmatrix} \tag{55}$$

$$B = \begin{bmatrix} 1 & & & & & & 1 & & & & & \\ & 1 & & & & & & & & & 1 & \\ & & 1 & & & 1 & & & & & & \\ 1 & & & & & & & & & & & 1 \\ & 1 & & & & & & & & & 1 & \\ & & 1 & & & & & & & 1 & & \\ & & & 1 & & & & & & & & 1 \\ & & & & 1 & & & & & & & 1 \\ & & & & & 1 & & & & & & 1 \\ 1 & & & & & & & & 1 & 1 & & \\ 1 & & & & & & & 1 & & & 1 & \\ 1 & & & & & & 1 & & & & & 1 \end{bmatrix} \quad \text{(All other elements are 0.)} \tag{56}$$

On the other hand, the vectors μ and $\mathbf{c}$ were chosen in two distinct ways. For the linear version $\mathbf{y} = A\mathbf{x} + \mu$ illustrated in Figs. 9 and 10

$$\mu = \begin{pmatrix} 0 \\ 3 \\ 6 \end{pmatrix}; \qquad \mathbf{c} = \mathbf{0} \tag{57}$$

while, for the linear-quadratic problem shown in Fig. 11

$$\mu = \mathbf{0}; \qquad \mathbf{c} = \begin{pmatrix} 1 \\ 2 \\ 3 \end{pmatrix} \tag{58}$$

With these particular choices, the exact means, variances and covariances for the elements of $\mathbf{y}$ are easily computed since, in this problem, $\mathbf{x}$ is a 12 vector of uncorrelated $N(0, 1)$ random variables so

$$\begin{aligned} E(x_i) &= 0 \\ E(x_i x_j) &= \delta_{ij} \\ E(x_i x_j x_k) &= 0 \\ E(x_i^2 x_j^2) &= 1 \end{aligned}$$

and

$$E(x_i^4) = 3 \tag{59}$$

For future reference, the results are:

	Linear Problem	Linear–Quadratic Problem
$E(y_1)$	0.0	3.0

$E(y_2)$	3.0	6.0
$E(y_3)$	6.0	9.0
$E(y_1^2)$	4.0	22.25
$E(y_2^2)$	46.0	119.0
$E(y_3^2)$	51.0	215.25
$E(y_1 y_2)$	2.0	38.5
$E(y_1 y_3)$	5.0	59.75
$E(y_2 y_3)$	27.0	136.5

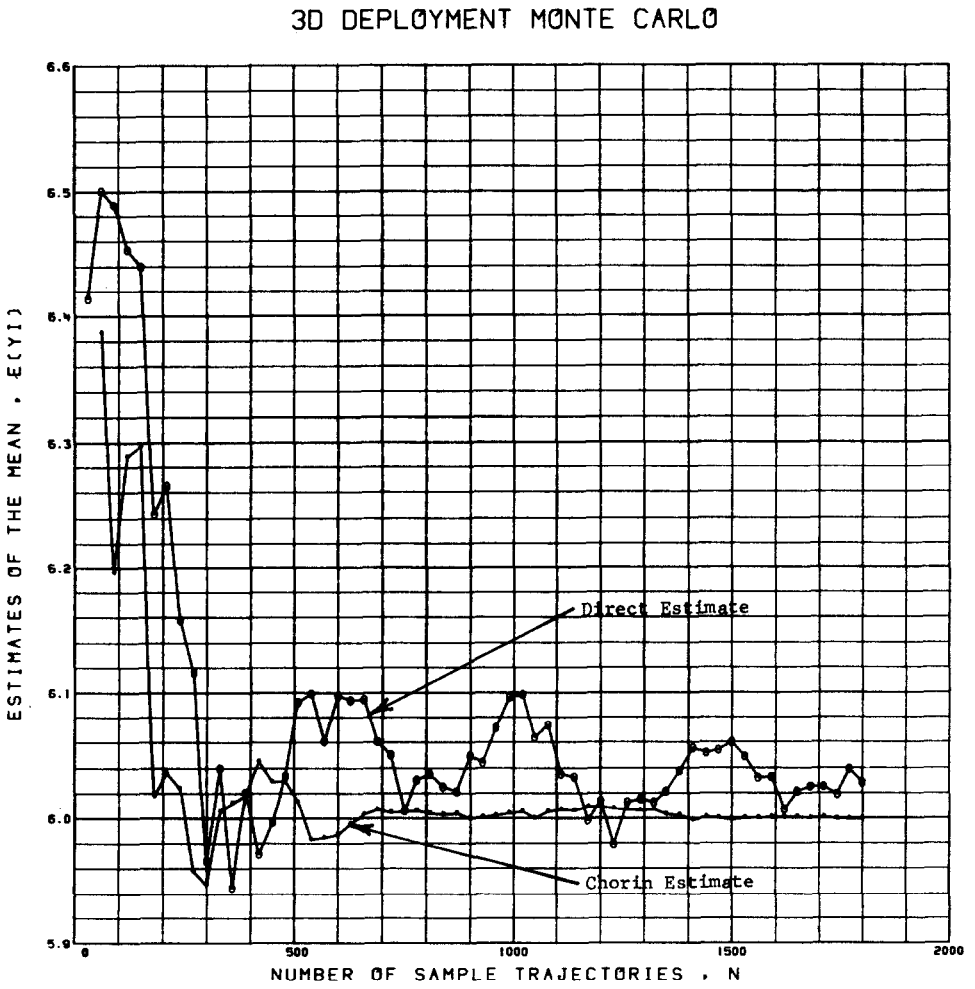

FIG. 10. Direct (○) and Chorin (*) estimates of the quantity y_3 for the deployment dispersion function $\mathbf{y} = A\mathbf{x} + \mu$ with $E[y_3] = 6$. The correction series here contains 11 terms.

Because of the simple structure of this problem, the exact Hermite series expansion can be constructed easily. As an example, consider

$$y_1 = x_1 + x_4 + x_7 + x_{10} \tag{60}$$

for the linear problem $\mathbf{y} = A\mathbf{x} + \boldsymbol{\mu}$. Since $n = 1$ is then the highest order polynomial to be retained in the expansion, $m = m(n, p) = m(1, 12) = 13$ is the full series length while, from (60), we see that only 5 terms are actually required. Similarly, for the linear-quadratic model illustrated in Fig. 11, the full series has $m = m(2, 12) = 91$ terms but, with exact correction, this is reduced to 36.

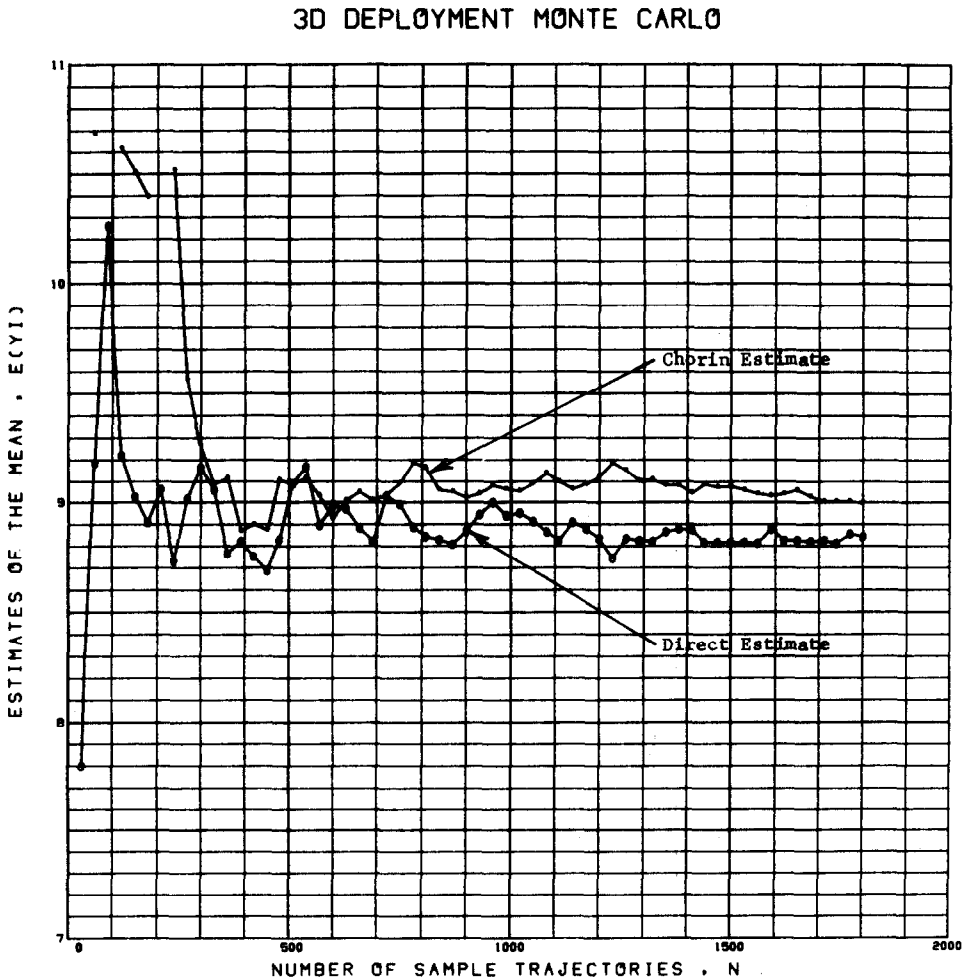

FIG. 11. Direct (○) and Chorin (*) estimates of the quantity y_3 for the deployment dispersion function $\mathbf{y} = A\mathbf{x} + \frac{1}{2}(\mathbf{x}^T B\mathbf{x})\mathbf{c}$ with $E[y_3] = 9$. As shown, this is a mixed linear-quadratic problem with a correction series of 36 terms.

As one can easily see from Figs. 9 to 11, the acceleration towards convergence is indeed dramatic. Furthermore, computations out to $N = 4000$ have shown that this behavior is uniformly and consistently maintained. Finally, fashioning the corrector series in advance to a specific problem then led to the idea of an Adaptive Series Selection Algorithm (ASSA) so that the same procedure could then be implemented automatically on the computer. This is discussed next.

Adaptive Series Selection

For problems of high dimensionality p, the basis set $\{\Phi_k\}$ of generalized orthonormal Hermite polynomials can become quite large if all the nonlinear interaction terms up to a given order n are included. Therefore, it is desirable to find some way of extracting a subset $\{\Phi_{k_i}\}$ which is not too large but which also approximates the function f quite well.

For purposes of illustration, we develop here a procedure using the basic Chorin estimator f^* with Monte Carlo error variance σ_C^2 given by

$$\sigma_C^2 = AM^{-1} + BM^{-2} \tag{61}$$

with $N = 2M$. First Eq. (61) is written in the more suggestive form

$$M\sigma_C^2 = \sigma^2 - \sum_{k=1}^{m} (a_k^2 - M^{-1}\sigma_k^2) \tag{62}$$

This is the equivalent single sample variance reduction (or increase!) with $M^{-1}\sigma_k^2$ the M-sample error variance for the coefficient estimate $\hat{a}_k$. Now (62) is again rewritten more compactly

$$M\sigma_C^2 = \sigma^2 - \sum_{1}^{m} \Delta_k \tag{63}$$

where

$$\Delta_k \triangleq a_k^2 - \sigma_{Mk}^2 \tag{64}$$

and

$$\sigma_{Mk}^2 \triangleq M^{-1}\sigma_k^2 \tag{65}$$

Note that Δ_k is then the single sample variance reduction associated with the kth term in the corrector series.

It is now obvious that, to optimize the selection of terms giving the subset maximizing variance reduction, one simply calculates N-sample Monte Carlo estimates $\hat{\Delta}_k$ and retains only these terms such that $\hat{\Delta}_k > 0$. The resulting error variance will be

$$\sigma_C^2 = M^{-1}\left(\sigma^2 - \sum{}^* \hat{\Delta}_k\right) \tag{66}$$

where the sum $\sum^*$ is over the index subset

$$\{k_i\,,\ 1 \leqslant k_i \leqslant m(n, p)\} \quad \text{such that} \quad \hat{\Delta}_{k_i} > 0.$$

The theoretical optimal subset $\{\Delta_{k_i}\}$ is referred to as the "variance reduction spectrum" since

$$\Delta_{k_i} = a_{k_i}^2 - \sigma_{Mk_i}^2 > 0 \tag{67}$$

The general problem of identifying and estimating the variance reduction spectrum as well as determining the errors in this procedure will be discussed in a future paper. Also, this leads to the further interesting idea of linear or nonlinear measure-preserving transformations of the random input vector $\mathbf{x}$

$$\mathbf{z} = S\mathbf{x} \qquad \text{or} \qquad \mathbf{z} = T(\mathbf{x}) \tag{68}$$

such that the variance reduction spectrum is focused as sharply as possible. In fact, initial calculations with the Deployment Dispersion Function have shown significant additional variance reduction after application of an appropriate measure-preserving transformation.

Computational Considerations

The basic Chorin estimator is linear in the trajectory solutions $f_i = f(\mathbf{x}_i)$, $i = 1, 2,..., N$ while the symmetric Chorin estimator is linear in $f_i = f(\mathbf{x}_i)$ and $f_i' = f(\mathbf{x}_i')$, $i = 1, 2,..., M$ with $N = 2M$. The tri-symmetric Chorin estimator is linear in $f_i = f(\mathbf{x}_i)$, $f_i' = f(\mathbf{x}_i')$ and $f_i'' = f(\mathbf{x}_i'')$, $i = 1, 2,..., M$ where $N = 3M$. These estimators all have the same general computational form, namely, they are linear weightings of the trajectory solutions. In these linear forms, the weighting coefficients are polynomial functions of the sample sets $S = \{\mathbf{x}_i\,,\ i = 1, 2,..., N\}$, $(S, S') = \{(\mathbf{x}_i\,,\ \mathbf{x}_i'),\ i = 1, 2,..., M = N/2\}$ and $(S, S', S'') = \{(\mathbf{x}_i\,,\ \mathbf{x}_i'\,,\ \mathbf{x}_i''),\ i = 1, 2,..., M = N/3\}$ for the three estimators f^*, f_{SC}^* and f_{TSC}^* respectively.

First considering the basic Chorin estimator, the linear form in f is obtained from Eq. (15) above as follows:

$$\begin{aligned} f^* &= \hat{f} - \sum_1^m \widehat{f\Phi_k'}\hat{\Phi}_k \\ &= \hat{f} - \overbrace{f\sum_1^m \Phi_k\hat{\Phi}_k}' \\ &= \sum_1^M (w_0 f_i + w_i' f_i') \end{aligned} \tag{69}$$

with the fixed weight $w_0 = M^{-1}$ and the variable weights $w_i' \triangleq -M^{-1}\sum_1^m \Phi_k(\mathbf{x}_i')\,\hat{\Phi}_k$ where $\hat{\Phi}_k \triangleq M^{-1}\sum_1^M \Phi_k(\mathbf{x}_i)$.

For a given class of problems (of dimensionality p), fixed Monte Carlo sampling scheme (N standard input samples with fixed proportioning) and fixed corrector series [maximum number of terms $m(n, p)$], there will be a unique set of weights $(w_0, \{w_i\})$ associated with this estimator. These weights can then be computed and stored for future use. This procedure is particularly efficient for parameter sensitivity analyses where repeated Monte Carlo runs are required under identical conditions except for the variability of the single parameter being investigated.

Similarly, for the symmetrized estimator f^*_{SC} given by

$$f^*_{SC} = \frac{f^*_1 + f^*_2}{2}, \tag{25}$$

we have

$$\begin{aligned} f^*_1 &= \sum_1^M (w_0 f_i + w'_i f'_i) \\ f^*_2 &= \sum_1^M (w_0 f'_i + w_i f_i) \end{aligned} \tag{70}$$

with $w_i \triangleq -M^{-1} \sum_1^m \Phi_k(\mathbf{x}_i)\, \hat{\Phi}'_k$ and w_0 and w'_i as defined above.

Thus, the symmetric Chorin estimator has the linear form

$$f^*_{SC} = \sum_1^M (v_i f_i + v'_i f'_i) \tag{71}$$

with the final (stored) weighting values

$$\begin{aligned} v_i &= \frac{w_0 + w_i}{2} \\ v'_i &= \frac{w_0 + w'_i}{2} \end{aligned} \tag{72}$$

Continuing for the tri-symmetric estimator f^*_{TSC} given by

$$f^*_{TSC} = \frac{f^*_1 + f^*_2 + f^*_3}{3} \tag{37}$$

with $N = 3M$, we now have

$$\begin{aligned} f^*_1 &= \sum_1^M (w_0 f_i + w'_i f'_i) \\ f^*_2 &= \sum_1^M (w_0 f'_i + w''_i f''_i) \\ f^*_3 &= \sum_1^M (w_0 f''_i + w_i f_i) \end{aligned} \tag{73}$$

The linear form for this estimator is

$$f^*_{TSC} = \sum_1^M (v_i f_i + v'_i f'_i + v''_i f''_i) \tag{74}$$

with the following (stored) weighting values

$$\begin{aligned} v_i &= \frac{w_0 + w_i}{3} \\ v'_i &= \frac{w_0 + w'_i}{3} \\ v''_i &= \frac{w_0 + w''_i}{3} \end{aligned} \tag{75}$$

For this estimator $w_0 = M^{-1}$ as before but the individual weights are

$$\begin{aligned} w_i &\triangleq -M^{-1} \sum_{k=1}^m \Phi_k(\mathbf{x}_i)\, \hat{\Phi}''_k \\ w'_i &\triangleq -M^{-1} \sum_{k=1}^m \Phi_k(\mathbf{x}'_i)\, \hat{\Phi}_k \\ w''_i &\triangleq -M^{-1} \sum_{k=1}^m \Phi_k(\mathbf{x}''_i)\, \hat{\Phi}'_k \end{aligned} \tag{76}$$

where

$$\begin{aligned} \hat{\Phi}_k &\triangleq M^{-1} \sum_{\alpha=1}^M \Phi_k(\mathbf{x}_\alpha) \\ \hat{\Phi}'_k &\triangleq M^{-1} \sum_{\alpha=1}^M \Phi_k(\mathbf{x}'_\alpha) \\ \hat{\Phi}''_k &\triangleq M^{-1} \sum_{\alpha=1}^M \Phi_k(\mathbf{x}''_\alpha) \end{aligned} \tag{77}$$

In each of the Eqs. (69), (71) and (74) for the three estimators, the fundamental weighting quantities all have the form

$$w_i = -M^{-1} \sum_1^m \Phi_k(\mathbf{x}_i)\, \hat{\Phi}'_k$$

where

$$\hat{\Phi}'_k = M^{-1} \sum_1^M \Phi_k(\mathbf{x}'_i)$$

There are recursion relations for Φ_k [see, for example, Eq. (7)] which could then be used to construct recursion relations for the intermediate component weights w_i. The final weights v_i, which are obtained from (72) and (75), can then either be used on-line or precomputed and stored for future use.

There is a trade between pre-stored weights and on-line generation of the weighting coefficients. This trade depends upon the available computer storage capacity and machine processing time required to generate each trajectory solution f_i. In general, if individual trajectories require a significant amount of machine time, the additional computer time needed for on-line generation of the weights w_i would be insignificant. On the other hand, for large scale, dedicated computer facilities, substantial overall speed advantages may be realized by using pre-computed weighting arrays prepared for different classes of problems.

CONCLUSIONS

In conclusion, these Hermite polynomial expansions are easy to manipulate, well-conditioned, and have good convergence properties. (Here, convergence is in the mean square error sense). Smoothing is consequently *global* rather than local as is characteristic of finite difference methods of numerical analysis. The exact reduction in Monte Carlo error depends upon how well the approximating Hermite series converges and how many individual terms are included in the series expansion. Furthermore, as is shown most clearly in Eqs. (40), there is a delicate interplay between *how important* a given term is in the resulting polynomial approximation to the estimand (net reduction in the mean-square remainder A) and *how accurately* the given term can be determined (net reduction in the sum of the coefficient error variances B).

For the Monte Carlo computer experiments, the principal purpose of the two models was to test numerically the variance reduction properties of various extended Chorin estimators. As one can easily see from the computational results shown in Figs. 6 and 8 to 11, this acceleration towards convergence can indeed be dramatic.

As a consequence of these significant reductions in Monte Carlo error, the use of orthonormal function space expansions is proposed as a bona-fide convergence acceleration device. This is a departure from conventional Monte Carlo computations since they have generally been considered to possess rather low precision and variance reduction devices have not been employed very often in actual practice.

ACKNOWLEDGMENTS

It is a sincere pleasure to thank Mr. Charlie Lee, Dan McGough, and Brad Wong of the Missile Systems Division (MSD) of Lockheed Missiles and Space Company for their long term interest and support of this work. Also we wish to thank Dr. Peter Hempel of MSD for initially suggesting the use of equidistributed random numbers. Finally, we are grateful to Mrs. Ramona Hague for her efforts in typing the final manuscript.

REFERENCES

1. W. FREIBERGER AND U. GRENANDER, "A Short Course in Computational Probability and Statistics," Applied Mathematical Sciences Series, Vol. 6, Springer–Verlag, New York, 1971
2. S. M. ERMAKOV, USSR Comput. Math. Math. Phys. **4** (1964), 213–219.
3. J. M. HAMMERSLEY AND D. C. HANDSCOMB, "Monte Carlo Methods," Methuen, London, 1964
4. P. J. DAVIS AND P. RABINOWITZ, "Methods of Numerical Integration," Academic Press, New York, 1975.
5. A. J. CHORIN, *J. Computational Phys.* **8** (1971), 472–482.
6. F. H. MALTZ AND D. L. HITZL, in preparation.
7. S. K. ZAREMBA, *SIAM Rev.* **10** (1968), 303–314.
8. R. H. CAMERON AND W. T. MARTIN, *Ann. of Math.* **48** (1947), 385–392.
9. F. H. MALTZ, *in* "Proceedings Sixth Symposium on Nonlinear Estimation Theory and Its Applications, San Diego, California, 1975."
10. F. H. MALTZ, *in* "Proceedings IEEE Conference on Decision and Control, New Orleans, Louisiana, 1977."
11. S. M. ERMAKOV AND V. G. ZOLOTUKHIN, *Theor. Probability Appl.* **5** (1960), 428–431.
12. D. C. HANDSCOMB, *Numer. Math.* **6** (1964), 261–268.