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VARIANCE REDUCTION IN MONTE CARLO ANALYSIS OF RAREFIED GAS DIFFUSION

by Morris Perlmutter
Lewis Research Center
Cleveland, Ohio

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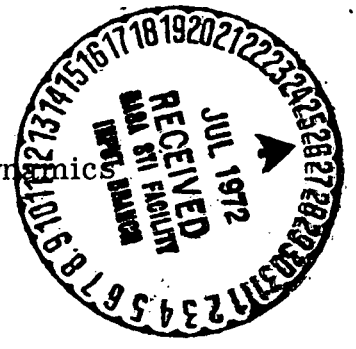

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VARIANCE REDUCTION IN MONTE CARLO ANALYSIS OF RAREFIED GAS DIFFUSION

by Morris Perlmutter

National Aeronautics and Space Administration
Lewis Research Center
Cleveland, Ohio

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The present analysis uses the Monte Carlo method to solve the problem of rarefied diffusion between parallel walls. The diffusing molecules are evaporated or emitted from one of two parallel walls and diffuse through another molecular species (see fig. 1). The M.C. analysis treats the diffusing molecule as undergoing a Markov random walk and the local macroscopic properties are found as the expected value of the random variable, the random walk payoff. By biasing the transition probabilities and changing the collision payoffs we can retain the expected Markov walk payoff but reduce its variance so that the M.C. result will have a much smaller error.

As shown in figure 1 the Markov random walk of the diffusing molecule can be represented by the sequence $\{X_o, X_1, X_2, \ldots\}$. X_n refers to a point in velocity and position space (V_n, Z_n) taken by the diffusing molecule immediately after the n^{th} collision. The probability density corresponding to this random walk is given by

$$H(X_o, X_1, \ldots)dX_o\, dX_1 \ldots = E_o(X_o)K(X_1|X_o)K(X_2|X_1), \ldots dX_o\, dX_1 \ldots \qquad (1)$$

The birth distribution $E_o(X_o)$ refers to the probability of the molecule originating at X_o. Assuming the molecules leaving the wall are in thermal equilibrium the birth distribution for the z component of the dimensionless velocity of the molecules leaving the wall is given by $E_o(v_{Zo}, Z = 0) = 2v_{Zo} \exp(-v_{Zo}^2)$. The transition probability $K(X_{n+1}|X_n)dX_{n+1}$ can be written as the product of a transport probability $T(Z_n \to Z_{n+1}|v_n)dZ_{n+1}$ and a collision probability $C(v_n \to v_{n+1}|Z_{n+1})dv_{n+1}$. The transport kernel T gives the probability of leaving Z_n and reaching Z_{n+1} at the $n+1$ collision while the collision kernel C gives the probability of a molecule at velocity v_n reaching a new velocity v_{n+1} after the $n+1$ collision. For the present model the transport kernel can be written in dimensionless form as $T(Z_n \to Z_{n+1}|v_n) = (1/|v_{Zn}|)\exp(-|Z_{n+1} - Z_n|/|v_{Zn}|)$. The collision kernel, assuming the molecules come out of collision with a Maxwellian distribution, will then not be a function of the previous velocity or position and can be written as $C(v_{Zn}) = (1/\sqrt{\pi})\exp(-v_{Zn}^2)$. We can write the event payoff after the n^{th} collision as $P(X_n)$. Then the payoff for the random walk η_o is given by

$$\eta_o = \sum_{n=0}^{\infty} P(X_n).$$

The expected value of the random walk payoff is given by

$$\lambda = \langle \eta_o \rangle = \int \cdots \int \left[\sum_{n=0}^{\infty} P(X_n) \right] E_o(X_o) K(X_1|X_o) K(X_2|X_1) \cdots dX_o \, dX_1 \cdots \quad (2)$$

The payoff term after each event can be written as $P(X_n) = p(v_n)\tau(Z_n \to Z_S|v_n)$. The $p(v)$ is some function of velocity of the molecule after a collision and $\tau(Z \to Z_S|v)$ is the scoring probability, the probability of the sample molecule reaching the scoring position Z_S from the last collision position without having another molecular collision. We can thus write $\langle \eta_o \rangle = n_S \langle p(v) v_Z \rangle_S / \mu_{o+}$; where n_S is the local molecular density at the scoring cross section and μ_{o+} is the molecular flux leaving the emitting surface. If the macroscopic quantity desired at the scoring position Z_S is the mass flux, μ_S, then $p(v)$ is given by $p_\mu = \pm 1$ for $v_Z \gtrless 0$. Similarly, if the local molecular number density n_S is desired at Z_S we have $p_n = \pm 1/v_Z$ for $v_Z \gtrless 0$. The scoring probability can be found to be $\tau(Z_n \to Z_S|v_{Zn}) = \exp(-|Z_n - Z_S|/|v_{Zn}|)$.

The potential payoff of a molecule leaving X_i is given by $\eta_i = P(X_i) + P(X_{i+1}) + \cdots$. Averaging this we can write the expected potential payoff conditional to leaving X_i as

$$W_i(X_i) = \langle \eta_i | X_i \rangle = \int \sum_{\ell=0}^{\infty} P(X_{i+\ell}) K_\ell(X_{i+\ell}|X_i) dX_{i+\ell}$$

$$= P(X_i) + \int W_{i+1}(X_{i+1}) K(X_{i+1}|X_i) dX_{i+1} \quad (3)$$

where

$$k_\ell(X_{i+\ell}|X_i) = \int \cdots \int K(X_{i+1}|X_i) \cdots K(X_{i+\ell}|X_{i+\ell-1}) dX_{i+1} \cdots dX_{i+\ell-1}.$$

We can similarly calculate the expected value of the square of the potential payoff of a molecule leaving X_i as

$$Q_i(X_i) = \langle \eta_i^2 | X_i \rangle = 2P(X_i)W_i(X_i) - P^2(X_i) + \int Q_{i+1}(X_{i+1}) K(X_{i+1}|X_i) dX_{i+1}$$

$$= \sum_{n=0}^{\infty} \int [2P(X_{i+n})W_{i+n}(X_{i+n}) - P^2(X_{i+n})] K_n(X_{i+n}|X_i) dX_{i+n} \quad (4)$$

The expected variance can now be written as

$$\sigma^2(\eta_o) = \int \langle \eta_o^2 | X_o \rangle E_o(X_o) dX_o - \langle \eta_o \rangle^2 = \int Q_o(X_o) E_o(X_o) dX_o - \langle \eta_o \rangle^2.$$

In the M.C. process we pick a birth velocity randomly from $E_o(v_o)$, then score $P(X_o)$. We then randomly choose the position of first collision from $K(X_1|X_o)$. We then score $P(X_1)$. The particle history is continued until it is incident on one of the walls. The payoff for the random walk is then given by η_o. This process is repeated for N samples. The expected payoff is then given by

$$\langle \eta_o \rangle \approx \bar{\eta}_o = \frac{1}{N} \sum_{i=1}^{N} \eta_{oi}$$

whose value is the desired macroscopic result appropriately representing the molecular flow rate or molecular density. The 95 percent confidence interval of $\bar{\eta}_o$ is given by

$$|\langle \eta_o \rangle - \bar{\eta}_o| \leq \epsilon = 1.96 \frac{\sigma(\eta_o)}{\sqrt{N}}$$

where $\sigma(\eta_o)$ is the standard deviation of η_o and can be obtained from the M.C. calculation by

$$\sigma^2(\eta_o) \approx \frac{1}{(N-1)} \sum_{i=1}^{N} \eta_{oi}^2 - (\bar{\eta}_o)^2$$

The analog M.C. calculation is the case in which the sample payoffs are given as $p(v)$ and are scored only when passing the scoring position. In table I the molecular density of the diffusing molecules at the scoring position $Z_S = \ell$ normalized by the density of the molecular flux emitted at $Z = 0$ is given under the heading "Analog." Also given are the results where the payoff is $p(v_n)\tau(Z_n \rightarrow Z_S | v_n) = P(v_n, Z_n)$. This is scored after each collision. These results are given under the heading "next event."

We wish to reduce the variance $\sigma(\eta_o)$ so that the error in the M.C. sampling will be smaller. To do this we bias the probabilities as follows. The probability of the biased walk is now given by $H^*(X_o, X_1, \ldots) = E_o^*(X_o)K^*(X_1|X_o)K^*(X_2|X_1)\ldots$. If we then distort the payoff to be

$$\eta = P(X_o) \frac{E_o(X_o)}{E_o^*(X_o)} + P(X_1) \frac{E_o(X_o)K(X_1|X_o)}{E_o^*(X_o)K^*(X_1|X_o)} + \ldots$$

We can see that the expected value of the random walk payoff is given by $\lambda^* = \int \cdot \int \eta_o^* H^* \, dX_o \, dX_1 \ldots = \lambda$ and is unchanged by the biasing process. A useful simplification is to write $K^*(X_{n+1}|X_n) = K(X_{n+1}|X_n)[I_{n+1}(X_{n+1})/I_n(X_n)]$. The biasing function must satisfy the usual probability normalization requirements. The probability density corresponding to the biased random walk is given by

$$H^* = [E_o(X_o)I_o(X_o)]\left[K(X_1|X_o) \frac{I_1(X_1)}{I_o(X_o)}\right]\left[K(X_2|X_1) \frac{I_2(X_2)}{I_1(X_1)}\right]\ldots$$

while the payoff for the random walk becomes

$$\eta_o^* = \frac{P(X_o)}{I_o(X_o)} + \frac{P(X_1)}{I_1(X_1)} + \frac{P(X_2)}{I_2(X_2)} + \ldots$$

For the biased case, the expected potential payoff for the random walk is given by $W_i^*(X_i) = [W_i(X_i)/I_i(X_i)]$.

Similarly, we can find the expected value of the potential square payoff for the biased random walk as

$$Q_i^*(X_i) = \frac{1}{I_i(X_i)} \sum_{n=0}^{\infty} \int [2P(X_{i+n})W_{i+n}(X_{i+n}) - P^2(X_{i+n})] \frac{K_n(X_{i+n}|X_i)}{I_{i+n}(X_{i+n})} dX_{i+n}$$

Since $\langle \eta_o^{*2} \rangle = \int E_o^*(X_o)Q_o^*(X_o)dX_o$ we can write the biased expected payoff as

$$\langle \eta_o^{*2} \rangle = \int \frac{E_o(X_o)}{I_o(X_o)} [2P(X_o)W_o(X_o) - P^2(X_o)]dX_o + \int \frac{E_1(X_1)}{I_1(X_1)} [2P(X_1)W_1(X_1) - P^2(X_1)]dX_1 + \int \frac{E_2(X_2)}{I_2(X_2)} [2P(X_2)W_2(X_2) - P^2(X_2)]dX_2 + \ldots \quad (5)$$

We wish to minimize $\langle \eta_o^{*2} \rangle$ with respect to $I_n(X_n)$ subject to the condition that

$$\int \cdots \int [E_o(X_o)I_o(X_o)] \left[K(X_1|X_1) \frac{I_1(X_1)}{I_o(X_o)}\right] \left[K(X_2|X_1) \frac{I_2(X_2)}{I_1(X_1)}\right] \ldots dX_o \, dX_1 \ldots = \int E_n(X_n)I_n(X_n)dX_n = 1 \quad (6)$$

Using the calculus of variations we find

$$\hat{I}_n(X_n) = \frac{[2P(X_n)W_n(X_n) - P^2(X_n)]^{1/2}}{\int E_n(X_n)[2P(X_n)W_n(X_n) - P^2(X_n)]^{1/2} dX_n} \quad (7)$$

Since $2P(X_n)W_n(X_n) - P^2(X_n) = Q_n(X_n) - \int Q_{n+1}(X_{n+1})K(X_{n+1}|X_n)dX_n$, this result implies that the importance function for the kernel biasing is proportional on the contribution to the variance of the molecules coming out of collision at X_n but not the future contribution to the variance from the later collisions. If we neglect higher order collision terms we can approximate the bias function by

$$\tilde{I}_n(X_n) = \frac{P(X_n)}{\int E_n(X_n)P(X_n)dX_n} \quad (8)$$

Now the transition kernels are biased so that more samples are taken with values that give larger contributions to the payoff. The biased payoff is now given by

$$P^*(X_n) = \frac{P(X_n)}{\tilde{I}_n(X_n)} = \int E_n(X_n)P(X_n)dX_n = \lambda_n \quad (9)$$

The payoffs are constant values for each event. This will reduce the variance of the random walk payoff.

The birth payoff is given by $P^*(X_o) = \lambda_o = \int E_o(X_o)P(X_o)dX_o$. This integral can be evaluated by numerical integration. Then a birth velocity can be randomly picked as usual and the unbiased procedure continued as before to find the next payoff $P(X_1)$. The result for this procedure is shown in table I labeled birth bias for the same cases as before.

We can continue the biasing to the first collision, $P^*(X_1) = \lambda_1 = \int E_o(X_o)K(X_1|X_o)P(X_1)dX_o\ dX_1$. However, it is difficult to evaluate λ_1 by numerical integration. Instead we can approximate the importance function by

$$\approx I_1(X_1) = \frac{P(X_1)}{\overline{T}_o(Z_o,v_o)\ \overline{CP}(Z_1)}$$

where $\overline{T}_o(X_o)$ is given by $\int_0^L T(Z_o \to Z_1|v_o)dZ_1$ and $\overline{CP}(Z_1) = \int_0^\infty C(v_1)P(v_1,Z_1)dv_1$. The payoff is then given by $P^*(X_1) = \overline{T}_o(v_o,Z_o)\overline{CP}(Z_1)$. To evaluate this we randomly choose v_o from $E_o(v_o)$ and Z_1 from $T(Z_o \to Z_1|v_o)/\overline{T}_o(X_o)$. With values for v_o and Z_1 we can then evaluate the first collision payoff $P^*(X_1)$. We can then continue the unbiased procedure retaining the v_o and Z_1. However since the Z_1 was found from the biased distribution the future payoffs must be weighted by $P^*(X_n) = P(X_n)\overline{T}_o(X_o)$. These results are shown in table I under +1 term bias.

This process can be continued to the second collision using

$$\approx I_2(X_2) = P(X_2)[\overline{T}_o(X_o)\overline{T}_1(X_1)\overline{CP}(Z_2)]^{-1} \qquad (11)$$

The $\overline{T}_1(X_1)$ is given by $\int_{Z_1}^{Z_L} (Z_1 \to Z_2|v_1)dZ_2$ where Z_L is L or 0 depending on $v_1 \lesseqgtr 0$. The payoff is then given by $P^*(X_2) = \overline{T}(X_o)\overline{T}(X_1)\overline{CP}(Z_2)$. To evaluate $P^*(X_2)$ we already have v_o and Z_1, we evaluate v_2 from $C(v_2)$ and Z_2 from $T(Z_1 \to Z_2|v_1)/\overline{T}_1(X_1)$. We can then evaluate the $P^*(X_2)$ payoff and we can continue either in the biased or unbiased fashion in this manner. The results for the biasing for three terms is shown in table I under +3 term bias.

Finally we can bias continuously, however in this case the sample history will not end because of the transport kernel biasing. The sample histories were then ended using Russian Roulette, samples were followed until the weighting $\overline{T}(X_o)\overline{T}(X_1)\ldots$ was less than 0.001, then if a randomly picked number, uniform between 0 and 1, was greater than 0.1 the history was ended, if less the sample weight was multiplied by a factor of 10 and the process continued. These results are in table I under Russian Roulette. The results indicate significant reductions in variance can be obtained using biased sampling techniques.

TABLE I. - NUMERICAL RESULTS

Sampling	Density ratio, n/n_{O+}	Mean deviation, σ	Time, min	Sampling	Density ratio, n/n_{O+}	Mean deviation, σ	Time, min
	10,000 Samples				10,000 Samples		
	$L/\lambda = 0.1$				$L/\lambda = 10$		
Analog	0.848	0.923	0.13	Analog	0.1202	0.578	2.14
Next event	.844	.867	.15	Next event	.11965	.527	2.33
Birth bias	.845	.741	.12	Birth bias	.11965	.527	2.31
+1 Term bias	.850	.1568	.42	+1 Term bias	.1171	.463	2.48
+3 Term bias	.855	.116	.64	+3 Term bias	.1195	.402	3.22
Russian Roulette	.854	.115	.61	Russian Roulette	.1172	.244	13.97
	$L/\lambda = 1$				$L/\lambda = 50$		
Analog	0.4914	0.7494	0.31	Analog	0.0261	0.224	10.78
Next event	.4881	.7188	.35	Next event	.0263	.238	11.61
Birth bias	.4881	.7185	.32	Birth bias	.0263	.238	11.60
+1 Term bias	.4958	.5728	.59	+1 Term bias	.0283	.2759	11.34
+3 Term bias	.487	.336	.95	+3 Term bias	.0246	.183	14.17
Russian Roulette	.491	.259	2.33	Russian Roulette	.0245	.168	39.50

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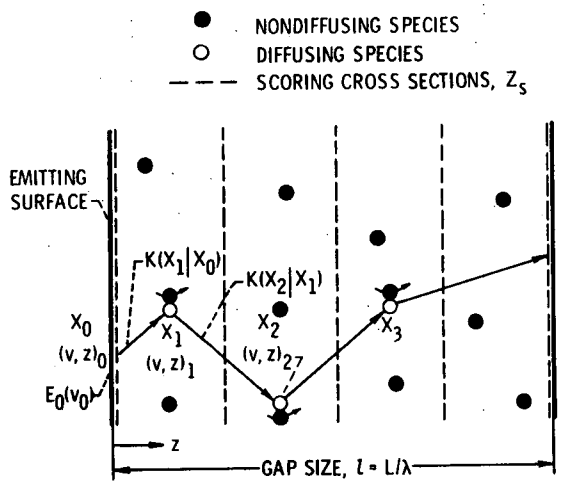

Figure 1. - Analytical model.