Letters to the Editor

On the Discrete Ordinates Method in Spherical Geometry

Reed and Lathrop[1] have made some suggestions for improving the solution of the transport equation in curved geometries by the discrete ordinates method. The suggestions are based on better representation of derivative terms. In the case of one-dimensional spherical geometry, the point $(r_{i+1/2}, \mu_m)$ at which the flux is evaluated is not necessarily the center of the phase-space cell. The particular choice of $r_{i+1/2}$ has been shown to reduce the truncation error of order $\Delta r^2/r^2$ to order $\Delta r^2/r$. This choice also removes the spurious flux dip at the center of a sphere. The choice of μ_m is also shown to be arbitrary as far as derivative terms are considered. This freedom is then used to choose some specific values of μ_m that can integrate quadratic polynomials correctly and thus satisfy the "diffusion condition." Such values of μ_m are shown to be away from the center of the angular cell by an amount of order $\Delta\mu^2$. Further, it has been shown that the truncation error with such a choice of μ_m is of order $\Delta\mu^2$, which is the same even when μ_m is chosen as a center.

Note that if certain requirements based on "neutron conservation" are used, the choice of μ_m is not arbitrary when one considers regions close to the center of a sphere. We find that it is preferable to use μ_m as the center of the angular cell. The requirement, in the words of Bell and Glasstone,[2] is "The difference equation for a fundamental (r, μ) cell should obey an explicit conservation law for neutron economy in that cell; each term in the equation should clearly represent a physical component in the neutron conservation, such as absorption or flow across a face." It is because of this requirement that the difference equation is derived from the "conservation form" of the transport equation so that the first term on the left side of Eq. (1) (given below) stands for net flow through physical faces and the second term stands for net flow through direction cell edges.

The difference equation is given by

$$\mu_m \frac{A_{i+1}N_{i+1} - A_iN_i}{V_{i+1/2}} + (A_{i+1} - A_i) \times \left(\frac{\alpha_{m+1/2}N_{m+1/2} - \alpha_{m-1/2}N_{m-1/2}}{V_{i+1/2}}\right) + \sigma N = S \ . \quad (1)$$

For the sake of simplicity and definiteness, let us consider the mesh closest to the center. Let $i = 0$ and $i = 1$ denote the center and edge, respectively, of this first mesh. Then A_0 is zero; therefore, the first term on the left side of Eq. (1) reduces to

$$E = [\mu_m A_1 N_1(\mu_m)]/V_{1/2} \ . \quad (2)$$

This term is expected to represent the flow of neutrons between $\mu_{m+1/2}$ and $\mu_{m-1/2}$ across the face of area A_1, according to the requirement stated above. Such a flow of neutrons can be rigorously expressed as

$$E^{exact} = \frac{1}{V_{1/2}(\mu_{m+1/2} - \mu_{m-1/2})} \cdot \int_{\mu_{m-1/2}}^{\mu_{m+1/2}} \mu \cdot A_1 \cdot N_1(\mu)\, d\mu$$

$$= \frac{A_1}{V_{1/2} \cdot \Delta\mu} \cdot \int_{\mu_{m-1/2}}^{\mu_{m+1/2}} \mu \cdot \left[N_1(\mu_m) + (\mu - \mu_m) \cdot \frac{\partial N_1}{\partial \mu}\bigg|_{\mu=\mu_m} + \frac{1}{2!}(\mu - \mu_m)^2 \cdot \frac{\partial^2 N_1}{\partial \mu^2}\bigg|_{\mu=\mu_m} + \ldots\right] d\mu \ . \quad (3)$$

We compare E and E^{exact} for the two choices of μ_m in the following.

Case 1: $\mu_m = \mu_{mean} = \dfrac{\mu_{m+1/2} + \mu_{m-1/2}}{2}$.

In this case it is easily seen that the leading term ΔE in $(E - E^{exact})$ is given by

$$\Delta E \approx \frac{A_1}{V_{1/2}} \cdot \frac{\partial N_i}{\partial \mu}\bigg|_{\mu=\mu_m} \cdot O(\Delta\mu^2) \ . \quad (4)$$

From the transport equation

$$\mu \cdot \frac{\partial N}{\partial r} + \frac{1 - \mu^2}{r} \cdot \frac{\partial N}{\partial \mu} + \sigma N = S \ , \quad (5)$$

it is obvious that $\partial N/\partial\mu$ tends to zero as fast as r tends to zero for physical problems. We note that for the first mesh under consideration, $A_1/V_{1/2}$ is of the order of $(1/\Delta r)$ and $r = \Delta r$. Therefore ΔE is of order $\Delta\mu^2$.

Case 2: $\mu_m = \mu_{mean} + O(\Delta\mu^2)$.

This is the choice suggested by Reed and Lathrop,[1] and it is seen that the leading term ΔE is

$$\Delta E \approx \frac{A_1}{V_{1/2}} \cdot N_1(\mu_m) \cdot O(\Delta\mu^2) \sim \frac{O(\Delta\mu^2)}{r} \ . \quad (6)$$

This difference ΔE is certainly large as compared to that in case 1 because r is small. Hence, it looks appropriate to use centrally placed μ_m in a few meshes close to the center. Near the

center, the angular flux tends to be isotropic, and it may not be necessary to choose μ_m as in case 2 in order to integrate quadratic polynomials exactly.

Thus the choice of $\mu_m = \mu_{mean}$ leads to a better representation of the neutron flow across the physical faces than the choice in case 2 near the center. Of course, the net flow across the faces of the phase-space cell, which is the sum of the first two terms on the left side of Eq. (1), may not be affected by the choice of μ_m in case 2. This can be easily seen in the light of the following relation:

$$\alpha_{m+1/2} - \alpha_{m-1/2} = -\omega_m \mu_m \ . \tag{7}$$

Nevertheless, the choice of μ_m, as in case 2, may lead to some incorrect redistribution of neutrons in angular and space variables. When regions away from the center are considered, the choice of μ_m is not so crucial. In that case, ΔE is obtained by replacing A_1 by $(A_{i+1} - A_i)$ in Eqs. (4) and (6). As $(A_{i+1} - A_i)/V_{i+1/2}$ is of order $(1/r)$ and $\partial N/\partial \mu$ need not tend to zero, it is seen for both cases that ΔE is of order $(\Delta \mu^2/r)$, which is small for large r.

R. S. Modak

Bhabha Atomic Research Centre
Reactor Analysis and Systems Division
Bombay - 400 085, India

October 31, 1984

REFERENCES

1. W. H. REED and K. D. LATHROP, *Nucl. Sci. Eng.*, **41**, 237 (1970).

2. G. I. BELL and S. GLASSTONE, *Nuclear Reactor Theory*, Van Nostrand Reinhold Company, New York (1970).

On Efficient Estimation of Variances

In Ref. 1 Dubi addresses the problem of the optimum estimation of variance from a given number of realizations of a random variable. The question is posed in the following way. Let $x_1, x_2, \ldots, x_n$ be independent realizations of the random variable x with an expectation μ and variance σ^2. Let the realizations be divided into groups ("batches") containing k realizations each and let

$$\bar{S}_i = \frac{1}{k} \sum_{j=1}^{k} x_{(i-1)k+j} \ . \tag{1}$$

If the variance of x is estimated in terms of the batchwise averages $\bar{S}_i$, what is the value of k that minimizes the variance of the estimated variance? In other words, what is the optimum batch size that gives the most reliable estimate of the variance? Dubi proves that *if the expectation μ of x is known, the optimum value of k is 1*, i.e. the "one-particle" estimation of the variance is the most reliable. He also shows that in the optimum case, the variance of the estimate is

$$D^2 = \frac{1}{n} \left[\langle (x-\mu)^4 \rangle - \langle (x-\mu)^2 \rangle^2 \right] \ , \tag{2}$$

where angle brackets stand for expectation.

In most practical cases, however, the expectation of the random variable is not known and therefore cannot be used in the estimation of the variance. In this letter we show that $k = 1$ is optimal also if the expectation is to be estimated, and this estimate is used in the estimate of the variance. It will also be shown that the variance of the entirely empirical estimate of the variance is higher than that in Eq. (2).

Let

$$\hat{S} = \frac{1}{p} \sum_{i=1}^{p} \bar{S}_i = \frac{1}{n} \sum_{i=1}^{n} x_i \ , \tag{3}$$

where $\bar{S}_i$ is the batchwise average in Eq. (1) and $p = n/k$, the number of batches formed from the n realizations. Obviously,

$$\langle \hat{S} \rangle = \mu \ ;$$

i.e., $\hat{S}$ is an unbiased estimate of the mean. Let

$$\bar{v}_i = \frac{n}{(p-1)} (\bar{S}_i - \hat{S})^2 \ ; \tag{4}$$

then it is easily seen that

$$\langle \bar{v}_i \rangle = \langle (x-\mu)^2 \rangle = \sigma^2 \ , \quad (j = 1, 2, \ldots, p) \ ;$$

i.e., $\bar{v}_i$ represents a realization of a random variable that has the expectation σ^2. The sample average formed from these realizations is

$$\hat{v} = \frac{1}{p} \sum_{i=1}^{p} \bar{v}_i \ , \tag{5}$$

which is obviously also unbiased with respect to σ^2. The question again is how to choose the value p (or equivalently the value of $k = n/p$) in order to minimize the variance of the estimate $\hat{v}$ in Eq. (5). The question is answered by calculating the variance in question. The variance of the estimate is

$$\hat{D}^2 = \langle \hat{v}^2 \rangle - \langle \hat{v} \rangle^2 = \left[\frac{n}{(p-1)} \right]^2 \left\langle \left[\frac{1}{p} \sum_{i=1}^{p} (\bar{S}_i - \hat{S})^2 \right]^2 \right\rangle - \sigma^4 \ . \tag{6}$$

The optimum value of $k = n/p$ with n given is the one that minimizes the quantity

$$Q(k) = \left[\frac{n}{(p-1)} \right]^2 \left\langle \left[\frac{1}{p} \sum_{i=1}^{p} (\bar{S}_i - \hat{S})^2 \right]^2 \right\rangle \ . \tag{7}$$

In order to make the derivations simpler, we introduce random variables with zero expectations. Thus, let

$$y = x - \mu \ , \quad y_i = x_i - \mu \ , \quad \bar{Z}_i = \bar{S}_i - \mu \ .$$

Then

$$\langle \bar{Z}_i \rangle = \langle \bar{Z}_i \bar{Z}_j \bar{Z}_r \bar{Z}_s \rangle = 0 \ , \quad (i \neq j, r, s) \ , \tag{8}$$

since the realizations x_i are assumed to be independent and therefore so are the sample averages $\bar{Z}_i$. Now, in view of Eqs. (1) and (3), the quantity in Eq. (7) reads

$$\begin{aligned} Q(k) &= \left[\frac{n}{p(p-1)} \right]^2 \left\langle \left[\sum_{i=1}^{p} \bar{Z}_i^2 - \frac{1}{p} \left(\sum_{i=1}^{p} \bar{Z}_i \right)^2 \right]^2 \right\rangle \\ &= \left[\frac{n}{p(p-1)} \right]^2 \left\langle \left(\frac{p-1}{p} \sum_{i=1}^{p} \bar{Z}_i^2 - \frac{1}{p} \sum_{i=1}^{p} \sum_{\substack{j=1 \\ j \neq 1}}^{p} \bar{Z}_i \bar{Z}_j \right)^2 \right\rangle \ . \end{aligned}$$

Explicit calculation of the square in brackets yields

$$Q(k) = \left[\frac{n}{p^2(p-1)} \right]^2 \left\langle (p-1)^2 \sum_{i=1}^{p} \bar{Z}_i^2 + [(p-1)^2 + 1] \times \sum_{i=1}^{p} \sum_{\substack{j=1 \\ j \neq 1}}^{p} \bar{Z}_i^2 \bar{Z}_j^2 \right\rangle \ ,$$