

VARIATIONAL VARIANCE REDUCTION FOR MONTE CARLO CRITICALITY PROBLEMS

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ABSTRACT

A previously-developed Monte Carlo Variational Variance Reduction (VVR) method is extended to estimate the k -eigenvalue of a multigroup neutronic system. The VVR method employs a variational functional that is theoretically more accurate than the direct functional used by traditional Monte Carlo calculations. While the direct functional requires an estimate of the forward flux only, the variational functional requires detailed estimates of both the forward and adjoint fluxes. The VVR method described in this paper employs a P_3 -in-angle, piecewise linear-in-space representation of the adjoint flux in each energy group; this is more accurate than representations used in previous VVR methods. The VVR method is more computationally expensive per particle than traditional Monte Carlo, due to the extra work required to evaluate the variational functional. However, with a class of multigroup, planar-geometry problems, we demonstrate that this increased cost is outweighed by a greater increase in accuracy, resulting in a significant gain in the figure of merit.

1. INTRODUCTION

Variational methods have recently been applied to Monte Carlo calculations in order to improve the accuracy of estimates of system characteristics, such as detector responses and eigenvalues (Allagi, 1998a), (Allagi, 1998b), (Barrett, 1998), (Barrett, 1999a), (Barrett, 1999b), (Barrett, 2001), (Densmore, 2000), and (Densmore, 2001). In these methods, a variational rather than a direct functional is used to provide an estimate of the system characteristic. Direct functionals, which are employed in traditional Monte Carlo calculations, require an estimate of the forward flux in the detector region only. Variational functionals, which are theoretically more accurate than direct functionals, require global estimates of the forward and adjoint fluxes. Recently, variational functionals have been employed in continuous space and angle

Monte Carlo calculations by (i) calculating the adjoint solution using a relatively inexpensive deterministic method, (ii) representing the adjoint flux as a function in phase space, and (iii) estimating the forward solution using Monte Carlo (Barrett, 1998), (Barrett, 1999a) (Barrett, 1999b), (Barrett, 2001), (Densmore, 2000), and (Densmore, 2001). We have called this general procedure Variational Variance Reduction (VVR).

The VVR method is more costly to implement per particle than traditional Monte Carlo, due to the extra work required to evaluate the variational functional. However, this extra computational expense is greatly outweighed by the accuracy gained by using the variational functional, yielding a much smaller variance and an increase in the figure of merit (FOM). In addition, the VVR method does not require nonanalog biasing, unlike standard variance reduction. However, the VVR method may be used with a nonanalog biasing scheme if it is advantageous to do so (Barrett, 1998), (Barrett, 1999a), (Barrett, 1999b), (Barrett, 2001), and (Densmore, 2000). In variance reduction techniques that employ a deterministically-calculated adjoint solution (Turner, 1997) and (Van Riper, 1997), the same adjoint flux may be used in evaluating the variational functional. This decreases the relative overhead cost of the deterministic calculation when these variance reduction methods are used in conjunction with VVR.

In recent work by us (Densmore, 2000) and (Densmore, 2001), the VVR method was used to treat planar-geometry, monoenergetic transport problems by representing the angular flux as a linear-in-angle, histogram-in-space or piecewise linear-in-space function. This procedure has two advantages over previous VVR implementations (Barrett, 2001): (i) it requires much less adjoint information to be stored; (ii) it is highly efficient for “diffusive” problems, due to the accurate representation of the angular flux. We have demonstrated that this VVR method improves the FOM of source-detector and eigenvalue problems. This improvement is especially evident in “diffusive” systems, where traditional variance reduction methods perform poorly.

In this paper, we extend this work to multigroup criticality problems. Also, we examine a P_3 (quartic) angular representation of the adjoint flux in the evaluation of the variational functional. Although this new VVR method requires additional adjoint information to be stored and additional forward information to be tallied, we show that the more accurate adjoint representation increases the FOM of the VVR method. In addition, the higher-order adjoint representation increases the types of problems in which the use of VVR is beneficial.

In the following, we describe the variational functional used to provide an estimate of the system eigenvalue, and we compare this functional to the direct functional employed by traditional Monte Carlo criticality calculations. We then discuss the representation of the adjoint flux and the implementation of the variational functional into a Monte Carlo variance reduction method. Finally, we demonstrate the

increase in FOM of the VVR method over traditional Monte Carlo for a class of planar-geometry, multigroup criticality problems.

2. THEORY

To describe this new VVR method, we consider the following 1-D, multigroup transport problem defined for $0 < x < X$, $-1 \leq \mu \leq 1$, and $1 \leq g \leq G$:

$$L\psi_g(x, \mu) = \frac{1}{k}F\psi_g(x, \mu) \quad . \quad (1)$$

Here the transport operator L is defined by

$$L\psi_g(x, \mu) = \mu \frac{\partial}{\partial x} \psi_g(x, \mu) + \Sigma_{tg}(x)\psi_g(x, \mu) - \frac{1}{2} \int_{-1}^1 \sum_{g'=1}^G \Sigma_{s,g' \rightarrow g}(x)\psi_{g'}(x, \mu') d\mu' \quad , \quad (2)$$

and the fission operator F is defined by

$$F\psi_g(x, \mu) = \frac{\chi_g(x)}{2} \int_{-1}^1 \sum_{g'=1}^G \nu \Sigma_{fg'}(x)\psi_{g'}(x, \mu') d\mu' \quad . \quad (3)$$

The relevant adjoint problem is:

$$L^*\psi_g^*(x, \mu) = \frac{1}{k}F^*\psi_g^*(x, \mu) \quad . \quad (4)$$

Here the adjoint transport operator L^* is defined by

$$L^*\psi_g^*(x, \mu) = -\mu \frac{\partial}{\partial x} \psi_g^*(x, \mu) + \Sigma_{tg}(x)\psi_g^*(x, \mu) - \frac{1}{2} \int_{-1}^1 \sum_{g'=1}^G \Sigma_{s,g \rightarrow g'}(x)\psi_{g'}^*(x, \mu') d\mu' \quad , \quad (5)$$

and the adjoint fission operator F^* is defined by

$$F^*\psi_g^*(x, \mu) = \frac{\nu \Sigma_{fg}(x)}{2} \int_{-1}^1 \sum_{g'=1}^G \chi_{g'}(x)\psi_{g'}^*(x, \mu') d\mu' \quad . \quad (6)$$

Appropriate vacuum or reflective boundary conditions apply to Eqs. (1) and (4). Although the transport problem specified above has isotropic scattering, the VVR method developed in this paper can easily be generalized to anisotropic scattering.

In traditional Monte Carlo, a simulation of Eq. (1) is performed to provide an estimate of the forward flux. This forward solution is then used to calculate the eigenvalue k by evaluating the direct functional

$$G[\Psi] = \frac{\langle 1, FL^{-1}F\Psi \rangle}{\langle 1, F\Psi \rangle} \quad . \quad (7)$$

Here we have used the inner product notation

$$\langle f, h \rangle = \int_0^X \int_{-1}^1 \sum_{g=1}^G f_g(x, \mu) h_g(x, \mu) d\mu dx \quad (8)$$

to imply integration over the entire phase-space domain of the problem. If Ψ is an estimate of the flux, then $F\Psi$ provides an estimate of the fission source, and $FL^{-1}F\Psi$ estimates the fission source in the next generation. Thus, Eq. (7) is the ratio of neutrons in successive generations. If the fission source is normalized to unity, as is commonly done in standard Monte Carlo calculations, then $\langle 1, F\Psi \rangle = 1$ and Eq. (7) reduces to the traditional estimator of k . Also, it is easy to verify that if $\Psi = \psi + \delta\psi$, then $G[\Psi] = k + O(\delta\psi)$.

In Monte Carlo calculations employing the VVR method, a Monte Carlo simulation of Eq. (1) is performed to provide an estimate of the forward flux, while a deterministic solution of Eq. (4) is calculated to provide an estimate of the adjoint flux. These solutions are then used to evaluate the variational functional

$$H[\Psi^*, \Psi] = \frac{\langle \Psi^*, F\Psi \rangle}{\langle \Psi^*, L\Psi \rangle} . \quad (9)$$

We now discuss several properties of the variational functional H . First, let us assume that Ψ and Ψ^* are estimates of the forward and adjoint fluxes of the form $\Psi = \psi + \delta\psi$ and $\Psi^* = \psi^* + \delta\psi^*$. Then, Eq. (9) can be written as

$$H[\Psi^*, \Psi] = k + \frac{\langle \psi^* + \delta\psi^*, F(\psi + \delta\psi) \rangle}{\langle \psi^* + \delta\psi^*, L(\psi + \delta\psi) \rangle} - \frac{\langle \psi^*, F\psi \rangle}{\langle \psi^*, L\psi \rangle} , \quad (10)$$

where the first and last terms of the right side of Eq. (10) cancel. Placing the second and third terms over a common demoninator, Eq. (10) yields

$$H[\Psi^*, \Psi] = k + \frac{\langle \psi^*, L\psi \rangle \langle \psi^* + \delta\psi^*, F(\psi + \delta\psi) \rangle - \langle \psi^*, F\psi \rangle \langle \psi^* + \delta\psi^*, L(\psi + \delta\psi) \rangle}{\langle \psi^*, L\psi \rangle \langle \psi^* + \delta\psi^*, L(\psi + \delta\psi) \rangle} . \quad (11)$$

Using Eq. (1), Eq. (11) becomes

$$H[\Psi^*, \Psi] = k + \frac{\langle \psi^* + \delta\psi^*, F(\psi + \delta\psi) \rangle - k \langle \psi^* + \delta\psi^*, L(\psi + \delta\psi) \rangle}{\langle \psi^* + \delta\psi^*, L(\psi + \delta\psi) \rangle} . \quad (12)$$

Collecting similar terms and using the definition of the adjoint operators, Eq. (12) can be rewritten as

$$H[\Psi^*, \Psi] = k + \frac{1}{\langle \psi^*, L\psi \rangle + O(\delta\psi^*) + O(\delta\psi) + O(\delta\psi^*\delta\psi)} [\langle \psi^*, F\psi \rangle + \langle \delta\psi^*, F\psi \rangle + \langle F^*\psi^*, \delta\psi \rangle - k(\langle \psi^*, L\psi \rangle + \langle \delta\psi^*, L\psi \rangle + \langle L^*\psi^*, \delta\psi \rangle) + O(\delta\psi^*\delta\psi)] . \quad (13)$$

Using Eqs. (1) and (4), all but the second-order error terms are eliminated from the numerator. Eq. (9) can finally be written as

$$H[\Psi^*, \Psi] = k + \frac{O(\delta\psi^*\delta\psi)}{\langle \psi^*, L\psi \rangle + O(\delta\psi^*) + O(\delta\psi) + O(\delta\psi^*\delta\psi)} . \quad (14)$$

Thus, the variational functional has the capacity to estimate k much more accurately than the direct functional. We also note that if the forward solution is calculated with Monte Carlo and the adjoint solution is calculated with a deterministic method, the asymptotic error after N samples can be written as

$$O(\delta\psi^*\delta\psi) = O(\delta\psi^*)O(\delta\psi) = \frac{O(\delta\psi^*)}{\sqrt{N}} \quad . \quad (15)$$

Thus, the VVR method is a true variance reduction method in the sense that it reduces the problem variance (by a factor related to the error in the deterministic adjoint calculation), but still converges as $1/\sqrt{N}$.

In addition, if one obtains an exact solution to either the forward or adjoint problem, it is easy to show that Eq. (9) yields

$$H[\Psi^*, \psi] = H[\psi^*, \Psi] = k \quad , \quad (16)$$

the exact eigenvalue. There are two interpretations of Eq. (16). First, if the Monte Carlo calculation yields an exact forward solution then the variational functional will yield the exact eigenvalue. Hence, in the limit of an infinite number of neutrons per generation and an infinite number of generations, the VVR method will calculate k exactly. Also, if one obtains an exact solution to the adjoint problem, then each Monte Carlo sample will yield the correct value of k with zero variance. In this case, the VVR method becomes a form of a zero-variance method in which the Monte Carlo calculation can be performed in analog, but the resulting information is combined with the adjoint solution in a nontraditional manner (Larsen, 2001). The VVR method differs from other zero-variance methods in the fact that it does not require a nonanalog Monte Carlo calculation to be performed.

3. IMPLEMENTATION

To implement the variational functional described above into a variance reduction method, we represent the deterministically-calculated adjoint flux estimate as a quartic-in-angle, piecewise linear-in-space function. This representation of the adjoint flux can be used to create a “reduced” functional, in which all terms can be completely estimated by the forward Monte Carlo calculation.

To calculate this adjoint flux representation, we subdivide the geometry into a “tally” grid $0 = x_{1/2} < x_{3/2} < \dots < x_{I+1/2} = X$, with constant material properties in each tally cell. Next, the tally grid is subdivided into a “fine” grid. We then use a deterministic method (discussed later) to approximate ψ^* on the spatial fine grid. The resultant fine-grid adjoint information is used to calculate the average Legendre moments in each tally cell $1 \leq i \leq I$ and energy group g :

$$\phi_{ngi}^* \equiv \frac{1}{\Delta x_i} \int_{x_{i-1/2}}^{x_{i+1/2}} \int_{-1}^1 P_n(\mu) \Psi_g^*(x, \mu) d\mu dx \quad , \quad 0 \leq n \leq 3 \quad . \quad (17)$$

Also, the average derivative of the adjoint scalar flux is calculated.

$$D\phi_{0gi}^* \equiv \frac{1}{\Delta x_i} \int_{x_{i-1/2}}^{x_{i+1/2}} \int_{-1}^1 \frac{\partial}{\partial x} \Psi_g^*(x, \mu) d\mu dx = \frac{\phi_{0g}^*(x_{i+1/2}) - \phi_{0g}^*(x_{i-1/2})}{\Delta x_i} . \quad (18)$$

Using the above information, the adjoint flux can be represented on the tally grid as the function

$$\Psi_g^*(x, \mu) \approx \sum_{n=0}^3 \frac{2n+1}{2} P_n(\mu) \phi_{ngi}^* + \frac{1}{2}(x - x_i) D\phi_{0gi}^* , \quad (19)$$

where $x_{i-1/2} < x < x_{i+1/2}$ and x_i is the center of cell i . Eq. (19) preserves the first four cell-average Legendre moments of the adjoint angular flux, and represents the zero-th moment (the adjoint scalar flux) as a piecewise linear function. We expect this quartic polynomial adjoint representation to be accurate for optically thick problems with high scattering ratios, more so than our previous work with linear angular representations of the adjoint flux (Densmore, 2000) and (Densmore, 2001). We also expect Eq. (19) to be accurate for less diffusive problems than our previous work, thus increasing the range of problems for which the use of the VVR method is advantageous.

Next, a Monte Carlo simulation of Eq. (1) is performed, and four angular moments of the forward cell-averaged angular fluxes are estimated:

$$\phi_{ngi} = \int_{x_{i-1/2}}^{x_{i+1/2}} \int_{-1}^1 P_n(\mu) \Psi_g(x, \mu) d\mu dx , \quad 1 \leq i \leq I , \quad 0 \leq n \leq 3 , \quad (20)$$

one spatial moment of the forward cell-averaged scalar flux is estimated:

$$M\phi_{gi} = \int_{x_{i-1/2}}^{x_{i+1/2}} \int_{-1}^1 (x - x_i) \Psi_g(x, \mu) d\mu dx , \quad 1 \leq i \leq I , \quad (21)$$

and four angular moments of the cell-edge angular fluxes are estimated:

$$\Gamma_{ngi} = \int_{-1}^1 \mu P_n(\mu) \Psi_g(x_{i-1/2}, \mu) d\mu , \quad 1 \leq i \leq I + 1 , \quad 0 \leq n \leq 3 . \quad (22)$$

The moments in Eqs. (20) and (21) are estimated by a track-length estimator, and the moments in Eq. (22) by a surface-crossing estimator. Note that Eq. (21) is just a line integral of the distance between the neutron position and the center of the cell along the neutron track. This integral can be evaluated as the average distance of the neutron from the center of the cell during the track weighted by the neutron track-length.

Introducing Ψ^* , represented by Eq. (19), into Eq. (9), we obtain a reduced functional that can be completely evaluated by a forward Monte Carlo calculation. To describe this reduced functional, we note that $H[\Psi^*, \Psi]$ can be written as

$$H[\Psi^*, \Psi] = \frac{\langle \Psi^*, F\Psi \rangle}{\langle \Psi^*, T\Psi \rangle + \langle \Psi^*, C\Psi \rangle - \langle \Psi^*, S\Psi \rangle} , \quad (23)$$

where the leakage operator T is defined by

$$T\psi_g(x, \mu) = \mu \frac{\partial}{\partial x} \psi_g(x, \mu) \quad , \quad (24)$$

the collision operator C is defined by

$$C\psi_g(x, \mu) = \Sigma_{tg}(x)\psi_g(x, \mu) \quad , \quad (25)$$

and the scattering operator S is defined by

$$S\psi_g(x, \mu) = \frac{1}{2} \int_{-1}^1 \sum_{g'=1}^G \Sigma_{s,g' \rightarrow g}(x) \psi_{g'}(x, \mu') d\mu' \quad . \quad (26)$$

Then, using Eqs. (20-22), the corresponding terms in the reduced functional can be expressed (without approximation to the forward problem) as the following:

$$\langle \Psi^*, F\Psi \rangle = \sum_{i=1}^I \sum_{g=1}^G \frac{\chi_{gi}}{2} \sum_{g'=1}^G \nu \Sigma_{fg'i} (\phi_{0gi}^* \phi_{0g'i} + D\phi_{gi}^* M \phi_{g'i}) \quad ; \quad (27)$$

$$\langle \Psi^*, C\Psi \rangle = \sum_{i=1}^I \sum_{g=1}^G \Sigma_{tgi} \left(\sum_{n=0}^3 \frac{2n+1}{2} \phi_{ngi}^* \phi_{ngi} + \frac{1}{2} D\phi_{gi}^* M \phi_{gi} \right) \quad ; \quad (28)$$

$$\langle \Psi^*, S\Psi \rangle = \sum_{i=1}^I \sum_{g=1}^G \frac{1}{2} \sum_{g'=1}^G \Sigma_{s,g' \rightarrow gi} (\phi_{0gi}^* \phi_{0g'i} + D\phi_{gi}^* M \phi_{g'i}) \quad ; \quad (29)$$

$$\begin{aligned} \langle \Psi^*, T\Psi \rangle &= \sum_{i=1}^I \sum_{g=1}^G \left[\sum_{n=0}^3 \frac{2n+1}{2} \phi_{ngi}^* (\Gamma_{ngi+1} - \Gamma_{ngi}) \right. \\ &\quad \left. + \frac{1}{2} D\phi_{gi}^* \left(\frac{\Delta x_i}{2} (\Gamma_{0gi+1} + \Gamma_{0gi}) - \phi_{1gi} \right) \right] \quad . \quad (30) \end{aligned}$$

In Eqs. (23) and (27-30), the adjoint information is obtained from a deterministic calculation via Eqs. (17) and (18), and the forward information is obtained from a Monte Carlo calculation via Eqs. (20-22). In this manner, the variational functional is completely estimated by a deterministic adjoint calculation and a Monte Carlo forward calculation.

When using the VVR method in performing a criticality calculation, generations of neutrons are followed as in traditional Monte Carlo. Neutrons in a given generation are tracked, and the resulting information is used to provide an estimate of k and source locations for the next generation (Lewis, 1993). However, in the VVR method the forward information collected in each generation is used to evaluate the variational functional as opposed to the direct functional. Thus, a variationally-calculated estimate of k is provided by each generation. These generation-wise estimates are then used to calculate a mean and a sample variance, as in traditional Monte Carlo.

Table 1: Fuel Cross-Sections

| g | Σ_{tg} | $\Sigma_{s,g \rightarrow g}$ | $\Sigma_{s,g \rightarrow g+1}$ | $\nu \Sigma_{fg}$ | χ_g |
|-----|---------------|------------------------------|--------------------------------|-------------------|----------|
| 1 | 0.1542 | 0.0663 | 0.0830 | 0.0096 | 0.575 |
| 2 | 0.3067 | 0.2455 | 0.0584 | 0.0012 | 0.425 |
| 3 | 0.5276 | 0.4326 | 0.0645 | 0.0177 | - |
| 4 | 0.9408 | 0.8198 | - | 0.1851 | - |

4. RESULTS

We now present results from a class of planar-geometry, multigroup criticality problems of the form of Eq. (1). These problems were run using the VVR method with (i) a linear (P_1) or quartic (P_3) angular representation of the adjoint solution, (ii) with and without the linear spatial term in Eq. (19), and (iii) using analog tracking or survival biasing (SB) in the forward Monte Carlo calculation. The results of these calculations are compared to a traditional Monte Carlo calculation, and the relative FOM (defined as their FOM divided by the traditional Monte Carlo FOM) is determined. The traditional Monte Carlo calculation used a track-length estimate of the direct functional and survival biasing. All calculations used 10,000 neutrons per generation, 225 total generations, and 25 generations were skipped to allow the fission source distribution to converge. The adjoint calculation was performed with a special-purpose finite difference P_3 code. In the problems considered in this paper, the Monte Carlo calculation took on the order of minutes of computer time, while all deterministic adjoint calculations took less than one second. Thus, we did not include the overhead cost of the adjoint calculation in the FOM. Although a P_3 code is used in this paper, the VVR method is easily used with any deterministic method in which moments of the angular flux can be calculated.

The first set of problems considered in this paper consist of alternating arrays of fuel and moderator regions, each region being 3.0 cm thick. The cross-sections for the fuel and moderator are given in Tables 1 and 2, respectively. Each problem is divided into a spatial grid $\Delta x = 1.0$ cm for the purposes of tallying the quantities in Eqs. (20-22). The relative FOM for these calculations are presented in Table 3. In addition, we have included a plot of the P_3 calculated thermal group forward scalar flux in Figure 1 for the largest problem. The fluxes in other groups and in other problems have a similar structure. The spatial dependence of the flux in Figure 1 illustrates the need for spatial resolution in our representation of the adjoint flux.

From Table 3, we see that the VVR method improves the FOM over traditional Monte Carlo. Note that moving from a P_1 to a P_3 angular representation and from a histogram to piecewise linear spatial representation also improves the efficiency of the VVR method, as expected. The largest improvement in the FOM comes from increasing the order of the angular flux representation. This improvement illustrates the importance of the angular accuracy over the spatial accuracy when approximating

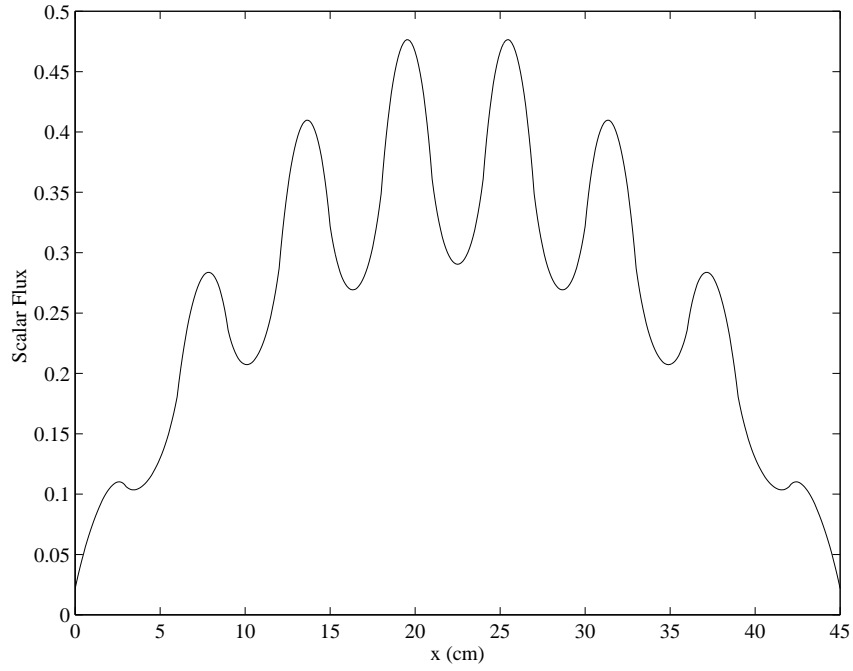


Figure 1: 8 Moderator, 7 Fuel Regions Thermal Flux

Table 2: Moderator Cross-Sections

| g | Σ_{tg} | $\Sigma_{s,g \rightarrow g}$ | $\Sigma_{s,g \rightarrow g+1}$ |
|-----|---------------|------------------------------|--------------------------------|
| 1 | 0.0698 | 0.0061 | 0.0636 |
| 2 | 0.2383 | 0.1467 | 0.0915 |
| 3 | 0.3749 | 0.2810 | 0.0938 |
| 4 | 1.5538 | 1.5409 | - |

Table 3: Array Problem Relative FOM

| VVR Method | 4 Moderator and 3 Fuel Regions | 6 Moderator and 5 Fuel Regions | 8 Moderator and 7 Fuel Regions |
|------------------|--------------------------------|--------------------------------|--------------------------------|
| P_1 | 18.8 | 25.6 | 31.1 |
| P_1 /SB | 11.0 | 14.3 | 18.3 |
| P_1 /Linear | 18.5 | 32.1 | 49.7 |
| P_1 /Linear/SB | 9.8 | 16.8 | 21.6 |
| P_3 | 113.8 | 108.2 | 123.4 |
| P_3 /SB | 60.6 | 101.9 | 100.9 |
| P_3 /Linear | 120.5 | 149.3 | 166.7 |
| P_3 /Linear/SB | 74.1 | 107.3 | 123.4 |

Table 4: Homogeneous Slab Problem Relative FOM

| VVR Method | 30 cm | 60 cm | 120 cm |
|------------------|-------|-------|--------|
| P_1 | 14.7 | 39.8 | 111.7 |
| P_1 /SB | 12.1 | 28.3 | 88.5 |
| P_1 /Linear | 28.9 | 128.3 | 981.4 |
| P_1 /Linear/SB | 15.7 | 77.7 | 401.5 |
| P_3 | 20.4 | 46.1 | 96.3 |
| P_3 /SB | 20.7 | 48.8 | 134.2 |
| P_3 /Linear | 64.3 | 415.7 | 3438.7 |
| P_3 /Linear/SB | 40.5 | 224.4 | 1816.0 |

the angular flux on the tally grid. We also note that the use of SB reduces the efficiency of the VVR method. However, using SB in conjunction with the VVR method still outperforms the traditional Monte Carlo calculation. The problems run with a P_3 angular representation and a piecewise linear spatial representation improved the FOM over the traditional Monte Carlo calculation by a factor greater than 100.

The next (simpler but less characteristic) set of problems considered are homogeneous slabs of fuel material only. Each problem is divided into a spatial grid $\Delta x = 5.0$ cm, again for the purposes of tallying the quantities in Eqs. (20-22). The relative FOM for these calculations are presented in Table 4.

From Table 4, we again see that the VVR method improves the FOM over traditional Monte Carlo for these slab calculations. As with the array problems, moving from a P_1 to a P_3 angular representation and from a histogram to piecewise linear spatial representation improves the efficiency of the VVR method. However, the largest improvement in the FOM in these problems comes from increasing the spatial order of the adjoint angular flux representation, not the angular order. Due to the diffusive nature of these problems, the exact adjoint solution is very nearly linear in both angle and space. Thus, improving the angular representation beyond linear results in little increase in accuracy, while representing the angular flux as a piecewise linear-in-space function is very accurate. In most cases, the use of SB with VVR reduces the efficiency of the eigenvalue calculation. However, in Table 4 the use of SB with the P_3 angular representation and histogram spatial representation actually improves the FOM. This improvement is most likely due to the larger variance in the higher angular moments. Even when SB is (non-optimally) used, the VVR method still outperforms the traditional Monte Carlo calculation. We note that in the largest problem in which the VVR method is used with a P_3 angular representation and a piecewise linear spatial representation, the FOM is improved over the traditional Monte Carlo calculation by a factor greater than 3000. This incredible improvement is due to the extremely accurate representation of the adjoint flux for this homogeneous

slab problem.

The above results illustrate the increased efficiency of the VVR method over traditional Monte Carlo. However, one may question if the resultant eigenvalue is biased by some truncation error, since the estimate of the adjoint flux is provided by a deterministic calculation. From Eqs. (14) and (15), the error in the variationally calculated eigenvalue becomes zero as the Monte Carlo-calculated forward flux becomes exact. The only effect of the truncation error in the adjoint flux is to decrease the error in the eigenvalue estimate. Thus, we expect the VVR method to provide an accurate estimate of the eigenvalue that is completely unbiased by any error in the adjoint flux.

To demonstrate the accuracy of the VVR method, the 30 cm homogenous slab problem was repeated with 30 different random number sequences using both a traditional Monte Carlo calculation and the VVR method (with a P_3 , linear-in-space adjoint representation). Each calculation used 500 neutrons per generation, 125 generations, and 25 generations skipped. The eigenvalue and standard deviation of these two sets of 30 trials were then compared to a traditional Monte Carlo benchmark consisting of 100,000 neutrons per generation, 2025 generations, and 25 generations skipped. From this comparison, it was determined if the benchmark calculation was within one trial standard deviation of the each trial eigenvalue. Of the 30 trials, 22 of the VVR method eigenvalues were within one standard deviation of the benchmark, while 15 of the traditional Monte Carlo eigenvalues met the same criteria. The Central Limit Theorem predicts that approximately 20 of the 30 trials should be within one standard deviation. Thus, for this sample problem, the VVR method provided a reasonably accurate estimate of the eigenvalue and standard deviation that agreed well with the predictions of the Central Limit Theorem.

Although the VVR method provides an accurate eigenvalue estimate with increased efficiency over traditional Monte Carlo, there are several difficulties in Monte Carlo criticality calculations relating to the estimation and use of the fission source. First, since the fission sites created in a previous generation are used as source sites in the next generation, the Monte Carlo estimates are correlated and their variances are inherently biased (Lewis, 1993). Thus, the VVR method underestimates the error in the eigenvalue, as traditional Monte Carlo does. Since relative FOM are calculated in this paper and this bias affects both the VVR method and traditional Monte Carlo, the results presented in this paper represent real improvement in the efficiency of the Monte Carlo calculation.

In addition to the difficulties in the estimation of variances in Monte Carlo criticality calculations, there is an inherent bias in the calculated eigenvalue in both the VVR method and traditional Monte Carlo due to the normalization of the fission source (Lieberoth, 1968). However, this bias is inversely proportional to the number of neutrons in each fission generation and is negligible for most problems employing a reasonable number of fission generations and neutrons per generation (Brissenden,

1986) and (Gelbard, 1994). The VVR method is further biased since the variational functional is a nonlinear functional of the forward flux. In general, the expected value of a ratio is not equal to the expected value of the numerator divided by the expected value of the denominator. This bias is also expected to become negligible as the number of neutrons per fission generation is increased. Also, we have not discussed difficulties with the convergence of the fission source, such as Whiteside’s “ k_{eff} of the World” problem (1971). However, as the same source sampling routine is used by both the VVR method and traditional Monte Carlo, both methods should be equally susceptible to source convergence problems.

5. CONCLUSIONS

We have described a variance reduction method for Monte Carlo eigenvalue problems in which adjoint fluxes are calculated deterministically, the forward fluxes are calculated using Monte Carlo, and the resultant information is used to evaluate a variational functional. This variational functional is theoretically more accurate than the direct functional used in traditional Monte Carlo calculations. Hence, the VVR method has the capacity to improve the FOM of eigenvalue calculations.

We have implemented this VVR method by representing the adjoint flux as a quartic-in-angle, piecewise linear-in-space function. This representation is extremely accurate for optically thick problems with high scattering ratios, and it increases the types of problems in which the use of the VVR method is advantageous over previous work. We have shown, with a class of multigroup, planar-geometry criticality problems, that the VVR method can significantly increase the FOM over traditional Monte Carlo calculations. We have also demonstrated that our adjoint representation is somewhat optimal, in the sense that the angular accuracy of the adjoint representation is more important than the spatial accuracy. Although we have limited our discussion to criticality problems, the methods described in this paper can be adopted to source-detector problems for diffusive systems as well. In future work, we plan to generalize this VVR technique to more practical multidimensional problems.

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REFERENCES

- Allagi, M.O., Lewins, J.D., and Parks, G.T., 1998a. “Variationally Processed Monte Carlo Transport Theory,” *Ann. Nucl. Energy*, **25**, 1055.
- Allagi, M.O. and Lewins, J.D., 1998b. “Real and Virtual Sampling in Variational Processing of Stochastic Simulation in Neutron Transport: The One-Dimensional Rod,” *Ann. Nucl. Energy*, **25**, 1521.

- Barrett, C.L. and Larsen, E.W., 1998. "A Variationally-Enhanced Monte Carlo Algorithm for Neutron Shielding Problems," *Trans. Am. Nucl. Soc.*, **79**, 166.
- Barrett, C.L. and Larsen, E.W., 1999a. "A Variational Variance Reduction Method for Monte Carlo Shielding and Eigenvalue Problems," Proc. ANS Topical Meeting: *Mathematics and Computation, Reactor Physics and Environmental Analysis in Nuclear Applications*, September 27 - 30, 1999, Madrid, Spain, **2**, 1371.
- Barrett, C.L., 1999b. "A Variationally-Based Variance Reduction Method for Monte Carlo Particle Transport Problems," Ph.D. Thesis, University of Michigan.
- Barrett, C.L. and Larsen, E.W., 2001. "A Variationally-Based Variance Reduction Method for Monte Carlo Neutron Transport Calculations," *Ann. Nucl. Energy*, **28**, 457.
- Brissenden, R.J. and Garlick, A.R., 1986. "Biases in the Estimation of k_{eff} by Monte Carlo Methods," *Ann. Nucl. Energy*, **13**, 63.
- Densmore, J.D. and Larsen, E.W., 2000. "A New Variational Variance Reduction Method for Monte Carlo Source-Detector Problems," *Trans. Am. Nucl. Soc.*, **83**, 336.
- Densmore, J.D. and Larsen, E.W., 2001. "Variational Variance Reduction for Monte Carlo Criticality Calculations," *Trans. Am. Nucl. Soc.*, submitted.
- Gelbard, E.M. and Gu, A.G., 1994. "Biases in Monte Carlo Eigenvalue Calculations," *Nuc. Sci. Eng.*, **117**, 1.
- Larsen, E.W. and Densmore, J.D., 2001. "New Zero-Variance Methods for Monte Carlo Criticality and Source-Detector Problems," *Trans. Am. Nucl. Soc.*, submitted.
- Lewis, E.E. and Miller, W.F. Jr., 1993. *Computational Methods of Neutron Transport*, American Nuclear Society, La Grange Park, Illinois.
- Lieberoth, J., 1968. "A Monte Carlo Technique to Solve the Static Eigenvalue Problem of the Boltzmann Transport Equation," *Nukleonik*, **11**, 213.
- Turner, S.A. and Larsen, E.W., 1997. "Automatic Variance Reduction for Three-Dimensional Monte Carlo Simulations by the Local Importance Function Transform - I: Analysis," *Nuc. Sci. Eng.*, **127**, 22.
- Van Riper, K.A., et al, 1997. "AVATAR - Automatic Variance Reduction in Monte Carlo Calculations," Proc. 1997 Joint International Conference on Mathematical Methods and Supercomputing for Nuclear Applications, Saratoga Springs, NY, **1**, 661.
- Whitesides, G.E., 1971. "A Difficulty in Computing k -effective of the World," *Trans. Am. Nucl. Soc.*, **14**, 680.