LA-UR-08-2837

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Intended for: PHYSOR-2008
Interlaken, Switzerland
14-19 September 2008

Los Alamos
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Dominance ratio calculations with MCNP

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Abstract

The dominance ratio quantifies the eigenvalue separation for reactor systems and is the key parameter in analyzing the convergence of iterative methods for solving criticality calculations. Two methods for calculating the dominance ratio have been tested in the MCNP Monte Carlo code – a new and potentially very accurate method based on time-series analysis, and the traditional but approximate fission matrix approach. Both methods have been tested on a variety of reactor and criticality safety problems.

1. Introduction

The dominance ratio of a multiplying system is defined as $DR=k_1/k_0$, where $k_0=k_{eff}$ is the eigenvalue of the fundamental mode and k_1 is the eigenvalue of the first higher mode. The dominance ratio is a fundamental property of a physical system and is a key parameter in analyzing system stability regarding fluctuations in xenon, voids, temperature, etc. Systems with a high dominance ratio (i.e., very close to 1.0) are more susceptible to oscillations induced by exciting a higher mode, while systems with a lower dominance ratio (DR<.9) are more stable with regard to fluctuations or disturbances in system parameters. This paper focuses, however, on a different role of the dominance ratio. When calculating k_{eff} and the power distribution for a reactor system, the dominance ratio is the key parameter for determining the convergence rate of an iterative numerical solution method. Monte Carlo eigenvalue calculations, for example, use the standard power method (Nakamura, 1986; Brown, 2005) for iteratively determining k_{eff} and the power distribution. For systems with a high dominance ratio, 100s or 1000s of iterations may be required before the method achieves convergence, while only 10s or 100s of iterations are required for systems with a low dominance ratio. Knowledge of the dominance ratio provides extremely valuable guidance to analysts performing the calculations: If it is known that the dominance ratio is close to 1.0, then convergence will be slow and special attention is required to avoid false convergence (i.e., misdiagnosis of convergence). If the dominance ratio is low, then the problem should converge quickly. For Monte Carlo eigenvalue calculations, assessment of convergence can sometimes be difficult due to the statistical nature of the calculations. If the cycle-to-cycle fluctuations in k_{eff} or the Shannon entropy of the source distribution (H_{src}) (Ueki and Brown, 2002; Brown, 2006) are large, problems with a high dominance ratio are more susceptible to false convergence. Knowledge of the dominance ratio would be especially helpful

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to Monte Carlo practitioners as an aid for assessing convergence.

2. Dominance ratio calculations

In the past, calculating the dominance ratio for criticality problems was generally left to deterministic power iteration methods. Some previous calculations using Monte Carlo methods involved calculating the fission matrix, and then determining the eigenvalues of the fission matrix. This approach suffers from both theoretical and computational drawbacks: The fission matrix is a discrete approximation to the physical problem. The infinite set of eigenvalues of the continuous problem is approximated by a smaller discrete set of eigenvalues, the number of which is equal to the number of discrete regions used in formulating the fission matrix. While the fundamental eigenvalue is identical to that of the continuous problem, all of the other eigenvalues of the fission matrix only approximate those of the continuous problem, approaching the correct values only in the limit of infinite dimension of the fission matrix. The requirement for a high dimensionality of the fission matrix creates computational problems. If the fission matrix is based on N regions, then N^2 storage elements are required for the fission matrix. Thus, a very crude 10x10x10 spatial mesh requires 10^6 storage elements for the fission matrix, and a 100x100x100 mesh would require an intractable 10^{12} storage elements. The Fission Matrix Method (FMM) for determining the dominance ratio must therefore be considered as only an approximate method, useful for obtaining "ball park" estimates. Nevertheless, the fission matrix method has been implemented in a test version of the MCNP5 Monte Carlo code (X-5 Monte Carlo Team, 2003). Convergence of the method as a function of the mesh size has been examined, and the results have been compared to a more accurate method discussed next.

Recently, an accurate method of determining the dominance ratio was developed for Monte Carlo eigenvalue calculations (Ueki et al., 2003; Ueki et al., 2004). This method was independent of bin structure and used time series analysis of a particular projection of the fission source vector to compute the dominance ratio. *DR* calculations were compared to exact benchmark results computed by Green's function methods. However, this method relied on the careful choice of bin boundaries to capture the symmetries of a system and on an autoregressive moving average (ARMA(2,1)) fit, which could be complicated and require fine tuning from the user. This method provided proof-of-principle and benchmark-quality results, but was primarily suitable for experts with prior knowledge of the fundamental and higher-mode solutions, rather than typical Monte Carlo code users.

An improvement to the ARMA(2,1) method was recently developed that retained the strengths of using time series analysis, but did not rely on the complicated ARMA fitting. This became the Coarse Mesh Projection Method (CMPM) (Nease and Ueki, 2007; Nease, 2008). This method was much the same as the previous one, but improved on the particular projection vector used. It was found that when using a certain projection vector, the dominance ratio could be computed reliably and robustly using a simple autoregressive order one (AR(1)) fitting. This method of calculating the dominance ratio has now been tested in the continuous-energy Monte Carlo code MCNP5 for a variety of realistic problems. Results have been compared to other methods of calculating the dominance ratio, including the approximate FMM.

3. CMPM for the dominance ratio

The CMPM for determining the dominance ratio has recently been described fully (Nease and Ueki, 2007; Nease, 2008), so only a brief summary is given here. The source eigenfunctions and eigenvalues of the transport equation, denoted by S_j and k_j are given by:

$$S_j(\vec{r}) = \frac{1}{k_j}\int S_j(\vec{r}')F(\vec{r}' \to \vec{r})dr' \qquad (1)$$

where k_j are ordered as $k_0 > k_1 > k_2 > \cdots$ and $F(\vec{r}' \to \vec{r})$ is the fission neutron kernel. For an iterative Monte Carlo calculation with N neutrons per cycle, the source for the m-th active cycle is represented as

$$\hat{S}^{(m)}(\vec{r}) = NS(\vec{r}) + \sqrt{N}\hat{e}^{(m)}(\vec{r}) \qquad (2)$$

where $\hat{e}^{(m)}(\vec{r})$ is the deviation from the true solution, dependent on the stochastic noise (from Monte Carlo histories) in each of the previous cycles, $\varepsilon^{(n)}(\vec{r}), \quad n = m, m-1, ..., 1$:

$$\hat{e}^{(m)}(\vec{r}) = \int A_0(\vec{r}' \to \vec{r}) \hat{e}^{(m-1)}(\vec{r}') dr' + \hat{\varepsilon}^{(m)}(\vec{r}) + O(N^{-1/2}) \quad (3)$$

where

$$A_0(\vec{r}' \to \vec{r}) \equiv \frac{1}{k_0} \left[F(\vec{r}' \to \vec{r}) - S_0(\vec{r}) \right] \quad (4)$$

In the CMPM, p coarse spatial bins (e.g., 2x2x2 mesh) are used to tally $\hat{e}^{(m)}(\vec{r})$ for each bin for a cycle, and then the noise-propagation matrix $\mathbf{A_0}$ is computed:

$$\begin{aligned} L_0 &= E\left[\vec{e}^{(m)} (\vec{e}^{(m)})^T \right] \\ L_1 &= E\left[\vec{e}^{(m+1)} (\vec{e}^{(m)})^T \right] \\ \mathbf{A}_0 &= L_1 L_0^{-1}. \end{aligned} \quad (5)$$

The eigenvalues and eigenvectors of $\mathbf{A}_0$ are then determined

$$\begin{aligned} \mathbf{A}_0 \vec{b}_i &= \lambda_i \vec{b}_i, \quad i, \ldots, p \\ \mathbf{A}_0^T \vec{d}_i &= \lambda_i \vec{d}_i, \quad i, \ldots, p \end{aligned} \quad (6)$$

and used as projection vectors to obtain an AR(1) estimate of the dominance ratio

$$DR = \frac{\sum_{m=2}^{M} \left(\vec{d}_1^T \cdot \vec{e}^{(m-1)} \right) \left(\vec{d}_1^T \cdot \vec{e}^{(m)} \right) \big/ \left(M-1 \right)}{\sum_{m=1}^{M} \left(\vec{d}_1^T \cdot \vec{e}^{(m)} \right)^2 \big/ M} \quad (7)$$

where M is the number of active cycles. The variance of the DR is estimated (for M cycles) by (Box et al., 1994):

$$\text{var}(DR) \approx \frac{1}{M}(1 - DR^2) \quad (8)$$

For the practical implementation of Eqs. 5-8 into MCNP5, it has been shown (Nease, 2008) that the equations can be recast in terms of $\hat{S}^{(m)}$ rather than $\vec{e}^{(m)}$, so that Eqs. 5 and 7 are replaced by

$$\begin{aligned} L_0' &= E\left[\hat{S}^{(m)} (\hat{S}^{(m)})^T \right] \\ L_1' &= E\left[\hat{S}^{(m+1)} (\hat{S}^{(m)})^T \right] \\ \mathbf{A}_0 &= L_1' L_0'^{-1} - I \end{aligned} \quad (9)$$

where I is the identity matrix, and

$$DR = \frac{\sum_{m=2}^{M} \left(\vec{d}_1^T \cdot \hat{S}^{(m-1)} \right) \left(\vec{d}_1^T \cdot \hat{S}^{(m)} \right) \big/ \left(M-1 \right)}{\sum_{m=1}^{M} \left(\vec{d}_1^T \cdot \hat{S}^{(m)} \right) \left(\vec{d}_1^T \cdot \hat{S}^{(m)} \right) \big/ M} \quad (10)$$

Thus, Eq. 9 is used in MCNP5 to determine the noise propagation matrix $\mathbf{A_0}$ based on the tallies of fission sources for each cycle, then any all-zero rows and columns of $\mathbf{A_0}$ are removed (i.e., $\mathbf{A_0}$ is reduced to span only fissionable regions), then the eigenvectors $\vec{d}_i$ from Eq. 6 are determined, and finally the DR is computed via Eq. 10. This approach results in a compact numerical scheme.

4. Numerical results

The FMM was implemented into MCNP5 in a straightforward manner, using the same mesh that is used for calculating the Shannon entropy of the source distribution (Brown, 2006). Given source neutrons in bin i, a tally of F_{ij} is made when a next-generation fission site is created in bin j. These tallies are accumulated over all cycles, converged or not. Periodically during the calculation, the eigenvalues of **F** (with columns normalized by the total fission neutron source in each region) are found and used to compute the dominance ratio. It should be noted that **F** is symmetric only for 1-group problems, and is nonsymmetric for general, energy-dependent problems. When **F** is large (e.g., 100s or 1000s of regions, with the size of **F** being the number of regions squared), finding the eigenvalues of a large, nonsymmetric matrix is a difficult numerical problem.

It should also be noted that statistical uncertainties were not determined for the DR computed with the FMM. There are 2 reasons for this: (1) As is well-known and will be demonstrated with the results below, the DR computed with the

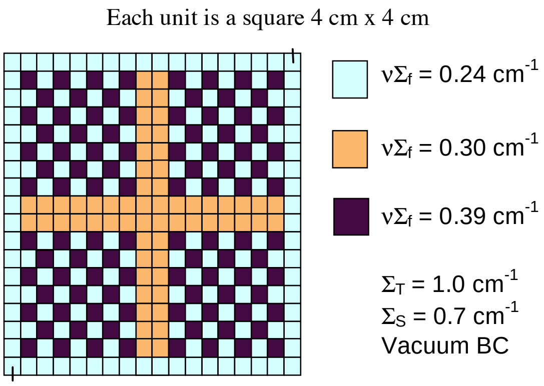

Fig. 1. 1-group 2D test problem

FMM is sensitive to discretization error and may be highly inaccurate if the mesh is too coarse. Providing statistics on wrong results is problematic; code users might be given the wrong impression. (2) The most serious difficulty with the FMM is the very large amount of computer memory storage required for an accurate (fine-mesh) fission matrix. Computing statistics would double the amount of storage required, hence intensifying the memory storage problem and limiting the FMM to even coarser meshes with larger discretization errors.

The tallies for the CMPM are also made on the same mesh used for the Shannon entropy, but are then collapsed to 2 bins in each direction (or 1 if the entropy mesh had only 1 bin in a direction). The CMPM tallies are only made for cycles after the iterations have converged. Equations (9), (6), and (10) are used at problem completion to determine the dominance ratio.

4.1. Results for Godiva test problem

For the very simple Godiva critical sphere, the sensitivity of the FMM approach to the spatial mesh is evident in the results shown in Table 1:

Table 1
DR results for the Godiva problem

	Mesh size	Matrix size	DR
FMM	2 x 2 x 2	8 x 8	.56
	4 x 4 x 4	64 x 64	.60
	8 x 8 x 8	512 x 512	.65
CMPM	2 x 2 x 2	8 x 8	.68 ± .03
ARMA(2,1) analysis			.63 ± .04

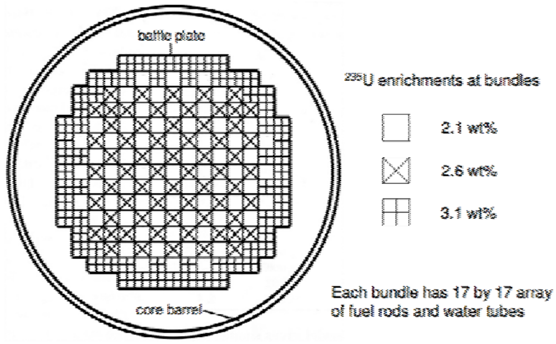

Fig. 2. 2D PWR initial core

In comparing results for the *DR* calculations, the ARMA(2,1) results are based on careful calculations according to the methodology described in (Ueki et al., 2003; Ueki et al., 2004) and are considered benchmark-quality results. The discretization error in FMM results is evident in Table 1, with the *DR* approaching the ARMA(2,1) *DR* as the mesh is refined. The CMPM result agrees with the benchmark within statistics.

4.2. Results for 1-group 2D test problem

For a 1-group 2D problem (Fig 1) with dominance ratio very close to 1, taken from (Ueki and Nease, 2006), results in Table 2 show a similar trend, with large FMM discretization errors for coarser meshes, and the CMPM result showing agreement with the benchmark ARMA(2,1) result.

Table 2
DR results for the 1-group 2D problem

	Mesh size	Matrix size	DR
FMM	4 x 4 x 1	16 x 16	.988
	9 x 9 x 1	81 x 81	.993
	18 x 18 x 1	324 x 324	.997
CMPM	2 x 2 x 1	4 x 4	.998 ± .002
ARMA(2,1) (Ueki and Nease, 2006)			.9993 ± .0004

4.3. Results for 2D PWR problem

A third problem, shown in Fig. 2, is a two-dimensional version of an initial PWR core as specified in (Nakagawa and Mori, 1993), with explicit geometry modelling of each fuel rod and water tube. The problem was analyzed using MCNP5 with reflecting top and bottom boundaries,

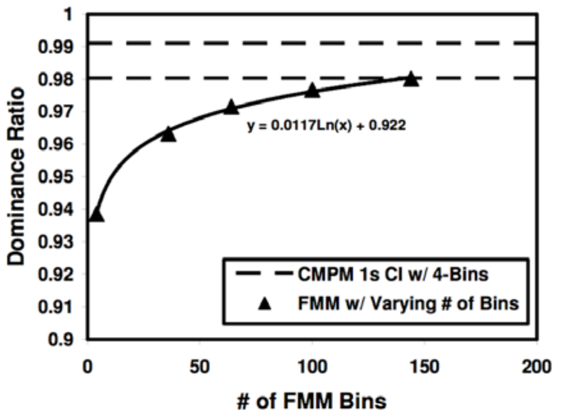

Fig. 3. DR by FMM for 2D PWR problem

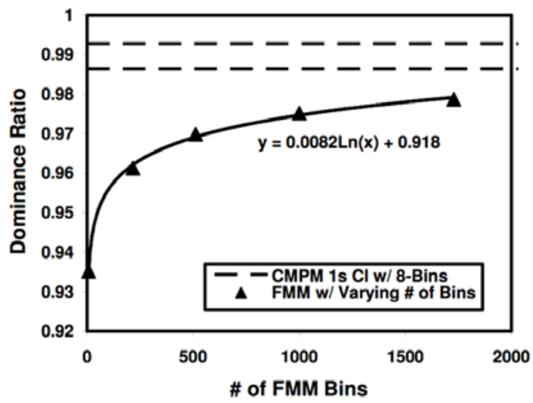

Fig. 4. DR by FMM for 3D PWR problem

and continuous-energy cross-section data. The CMPM analysis runs used 200,000 neutrons per cycle, 1,000 inactive cycles, 9,000 active cycles, and a 2x2x1 spatial mesh (4 bins) for the CMPM analysis. As shown in Table 3, the CMPM yields accurate results for the *DR*.

Table 3
DR results for the 2D PWR problem

	Mesh size	Matrix size	DR
CMPM	2 x 2 x 1	4 x 4	.991 ± .003
ARMA(2,1) (Nease and Ueki, 2007)			.993 ± .002

Fig. 3 shows how the *DR* computed by the FMM for this problem varies as a function of the number of spatial bins. For the FMM, the *DR* results are not reliable unless a mesh with at least 12x12x1 bins is used, requiring a 144x144 element fission matrix.

4.4. Results for 3D PWR problem

When the PWR problem of Nakagawa and Mori (1993) is run as originally specified with 3D geometry, including the plenum, top and bottom end plugs, and top and bottom supports, the FMM difficulty with memory storage vs accurate results become strikingly apparent. Fig. 4 shows that with a 12x12x12 mesh, giving 1728 FMM bins and 2,985,984 matrix elements, the *DR* computed with the FMM is seriously in error.

4.5. Results for 1D heterogeneous slab problem

This test problem is a simple, 1-group, multi-region slab geometry problem with vacuum boundaries, shown in Fig. 5. The *DR* was previously computed with a highly-accurate Green's Function method (Kornreich, 2003) using an 1,800-bin mesh. This problem verifies that the CMPM can yield accurate *DR* results even when the *DR* is very close to 1, *DR* ~ $.999^{+}$. Table 4 gives the benchmark Green's Function and CMPM results, showing excellent ageement. The CMPM used 80,000 neutrons per cycle, 400 inactive cycles, and 40,000 active cycles.

Table 4
DR results for the 1D slab problem

	Mesh size	Matrix size	DR
Green's Function	1800		.999565
CMPM	2 x 1 x 1	2 x 2	.9994 ± .0003

5. Additional considerations for CMPM

5.1. Number of cycles for DR calculations

The basis for the CMPM is an accurate estimation of the noise-propagation matrix $\mathbf{A_0}$, given by Eq. 5 or Eq. 9. Elements of $\mathbf{A_0}$ are constructed from the covariances among fission sources for each tally bin over the active problem cycles. Hence, sufficient cycles must be run to reliably estimate the

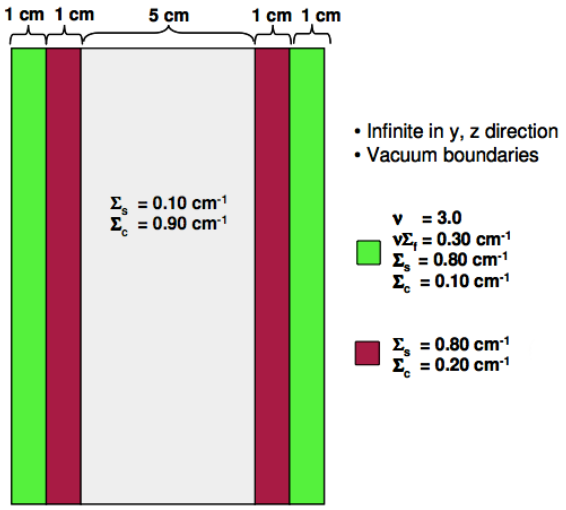

Fig. 5. 1D slab test problem

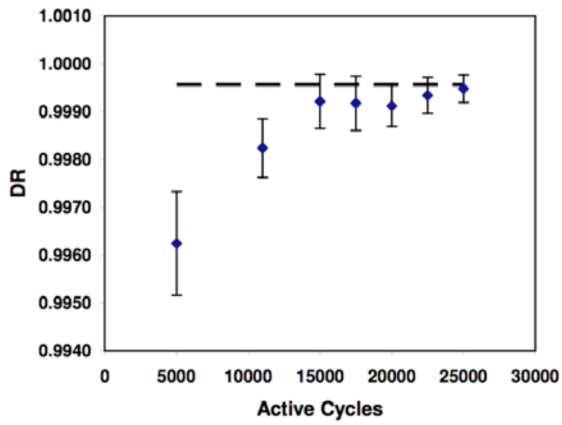

Fig. 6. *DR* from CMPM vs active cycles, for 1D slab test problem

covariances among the fission source tally bins. For problems with high *DR*, however, it is well known that the fission source tallies for each cycle are highly correlated (Brown, 2005). As discussed in (Nease, 2008), these correlations decay roughly as DR^m, where m is the number of active cycles. To ensure that sufficient cycles are used to account for the correlations when determining the covariances required for $\mathbf{A_0}$, we suggest that enough cycles be run so that $DR^m < 0.1\%$. That is, enough active cycles should be run that there is less than about 0.1% correlation between the first and last active cycle. This ansatz results in the condition

$$M_{\min} = \frac{\ln 0.001}{\ln DR} \tag{11}$$

where M_{min} is the minimum number of active cycles that should be run.

Fig. 6 shows the DR computed by the CMPM for the 1D slab test problem (Fig. 5) as a function of the number of active cycles used. This problem, with the actual *DR*=.999565, is an extreme case, where Eq. 11 predicts that about 16,000 active cycles are necessary to reduce correlation effects to <0.1%. The prediction of Eq. 11 with the actual results shown in Fig. 6 is excellent.

Two applications of Eq. 11 are possible: First, the approximate *DR* from the FMM could be used early in a calculation to estimate the number of active cycles needed for the CMPM. Second, after the CMPM calculation, Eq. 11 could be used as a diagnostic for the reliability of the computed *DR*.

5.2. Numerical issues

In applying the CMPM, it is necessary to determine the eigenvalues and eigenvectors of the noise propagation matrix, $\mathbf{A_0}$, given by Eq. 9. $\mathbf{A_0}$ will in general be nonsymmetric, even for 1-group problems. As such, the eigenvalues of $\mathbf{A_0}$ cannot be guaranteed as real, and numerical roundoff could lead to complex eigenvalues. Further, due to the noise introduced in $\mathbf{A_0}$ by the Monte Carlo statistical fluctuations, there is a greater possibility of obtaining complex higher eigenvalues. Such complex higher eigenvalues have indeed been observed in some of the test problems reported in (Nease, 2008).

It was observed in (Nease, 2008) that complex parts to the higher eigenvalues occurred more frequently for degenerate eigenvalues (or near-degenerate); that the magnitude of the complex parts was small relative to the real parts; that the magnitude of the complex parts decreased when more active cycles were used; that the decrease in magnitude of the complex parts was bounded by M^{-1} and $M^{-1/2}$, where M is the number of active cycles; and that complex parts generally occurred for 2nd, 3rd, or higher eigenvalues and not for the 1st, the *DR*.

After much investigation, testing, and comparison to accurate benchmarks, it was determined (Nease, 2008) that the CMPM will produce accurate *DR* results even in the presence of small complex parts to higher eigenvalues, so long as the real part of the projection vector $\vec{d}_1$ is used in Eq. 10 for determining the *DR*.

5.3. Computation times

Because the CMPM is free of discretization error, a coarse mesh can be used, with just 2 intervals in each coordinate direction. Typically the sizes of the $\mathbf{A_0}$ matrix are 2x2 for 1D problems, 4x4 for 2D problems, and 8x8 for 3D problems. Accordingly, the computer memory storage and additional CPU time for the CMPM is negligible compared to the time for running the Monte Carlo histories. In (Nease, 2008), some test problems were run using more mesh intervals, primarily for determining additional higher mode eigenvalue ratios, k_2/k_0, k_3/k_0, etc.

6. Conclusions

Two methods for calculating the dominance ratio have been implemented into a test version of MCNP5. The fission matrix method is approximate, but has the advantage that it yields a rough estimate of the dominance ratio early in a calculation, even before a problem has converged. The coarse-mesh projection method provides an accurate estimate of the dominance ratio, but can be used only after a calculation has converged. Both methods are robust and require little or no user intervention. Testing has being carried out on a variety of reactor and criticality safety problems. Given the continued success of the methods, both will be made available in forthcoming production versions of MCNP.

Knowledge of the dominance ratio should be a very useful aid to Monte Carlo practitioners for assessing convergence. In addition, knowledge of the dominance ratio may be useful in deriving automated tests for convergence during the Monte Carlo calculations.

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