LA-UR-03-0106

*Approved for public release;
distribution is unlimited.*

Title:

DOMINANCE RATIO COMPUTATION VIA TIME SERIES ANALYSIS OF MONTE CARLO FISSION SOURCES

Author(s):

Taro Ueki, Forrest B. Brown, D. Kent Parsons

Submitted to:

American Nuclear Society 2003 Annual Meeting,
San Diego, CA, June 1-5, 2003

Los Alamos
NATIONAL LABORATORY

DOMINANCE RATIO COMPUTATION VIA TIME SERIES ANALYSIS OF MONTE CARLO FISSION SOURCES

Taro Ueki, Forrest B. Brown and D. Kent Parsons

Applied Physics Division, Los Alamos National Laboratory, MS F663, Los Alamos, NM 87545

INTRODUCTION

Error propagation of Monte Carlo (MC) fission source distribution through iteration cycles is a noise-driven linear Markov process when the number of histories per iteration cycle is sufficiently large [1]. We show that the discrete version of such a Markov process combined with linear observation functions has an autoregressive moving average (ARMA) representation. Since ARMA processes are standard stochastic models in time series analysis, one can attempt at ARMA fitting to compute physical and statistical parameters relevant to criticality analysis. In this article, we demonstrate the application of ARMA fitting to dominance ratio computation.

ERROR PROPAGATION OF MC FISSION SOURCE AND TIME SERIES ANALYSIS

We show how the results of previous work on the error propagation of MC fission source [1] can be cast into time series analysis. Let $F(\vec{r}' \to \vec{r})$ be the expected number of the first generation descendant particles per unit volume at $\vec{r}$ resulting from a particle born at $\vec{r}'$. In the case of a position independent energy spectrum, $F(\vec{r}' \to \vec{r})$ is the fission kernel defined by the product of energy and angular spectrums, an inverse transport operator and a fission operator, with the last operator defined as $\int\int \nu\Sigma_f(\vec{r},E)\psi(\vec{r},E,\vec{\Omega})d\Omega dE$ for the operand ψ and the fissile descendent generation cross section $\nu\Sigma_f$. The eigenfunctions and eigenvalues of F are denoted by S_j and k_j:

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

where k_j are ordered as $k_0 > |k_1| > |k_2| > \cdots$. The eigenvalue k_j's are assumed to be discrete. Note that k_{eff} is the largest eigenvalue k_0 and S_0 is called the fundamental mode eigenfunction and assumed to be normalized to k_0:

$$\int S_0(\vec{r})dr = k_0 = k_{eff}. \qquad (2)$$

The normalization condition (2) cannot generally be assumed for S_j, $j \ge 1$ because in symmetric problems eigenfunctions may integrate to zero for some of the non-fundamental modes. In order to simplify later derivations, the following normalization scheme is imposed on the nonfundamental mode eigenfunctions:

$$S_j(\vec{r}) \leftarrow \frac{k_j S_j(\vec{r})}{\int S_j(\vec{r})dr} \text{ when } \int S_j(\vec{r})dr \ne 0, \qquad (3)$$

i.e., the whole domain integral of $S_j(\vec{r})$ is normalized to the corresponding eigenvalue as far as $\int S_j(\vec{r})dr \ne 0$ and no specification is made otherwise. The source (distribution of fission sites) after simulating the m-th stationary cycle in a MC criticality calculation is written as

$$\hat{S}^{(m)}(\vec{r}) = NS(\vec{r}) + \sqrt{N}\hat{e}^{(m)}(\vec{r}),\ m \ge 0, \qquad (4)$$

where $\hat{e}^{(m)}(\vec{r})$ is the fluctuating component of the stationary source, N the number of particle histories per cycle, the hats indicate a realization of stochastic quantities, and $S(\vec{r})$ is the expected value (ensemble average) of $\hat{S}^{(m)}(\vec{r})/N$. In addition, the random noise component $\hat{\varepsilon}^{(m)}(\vec{r})$ resulting from the starter selection and subsequent particle tracking can be introduced as

$$\sqrt{N}\hat{\varepsilon}^{(m)}(\vec{r}) \equiv \hat{S}^{(m)}(\vec{r}) - \frac{N\int F(\vec{r}' \to \vec{r})\hat{S}^{(m-1)}(\vec{r}')dr'}{\int \hat{S}^{(m-1)}(\vec{r}'')dr''} \qquad (5)$$

The fluctuating part of MC fission source then becomes a linear Markov process driven by uncorrelated noises with the nonlinear terms with the order of $O(N^{-1/2})$ [1]:

$$\hat{e}^{(m)}(\vec{r}) = A_0\hat{e}^{(m-1)}(\vec{r}) + \hat{\varepsilon}^{(m)}(\vec{r}) + O(N^{-1/2}), \qquad (6)$$

$$E[\hat{\varepsilon}^{(p)}\hat{\varepsilon}^{(q)}]=0,\ p>q, \tag{7}$$

where A_0 is defined as

$$A_0(\bullet)=\frac{1}{k_0}\int\left[F(\vec{r}\,'\to\vec{r})-S_0(\vec{r})\right](\bullet)dr' \tag{8}$$

The operator A_0 has the following interesting properties:

$$A_0^{\,i}S_0(\vec{r})=0 \quad \text{for } i\ge 1, \tag{9}$$

$$A_0^i\left[S_j(\vec{r})-S_0(\vec{r})\right]=\left(\frac{k_j}{k_0}\right)^i\left[S_j(\vec{r})-S_0(\vec{r})\right] \quad \text{for } j\ge 1 \text{ with } \int S_j(\vec{r})dr\ne 0\ \ j\ge 1, \tag{10}$$

$$A_0^iS_j(\vec{r})=\left(\frac{k_j}{k_0}\right)^i S_j(\vec{r}) \quad \text{for } j\ge 1 \text{ with } \int S_j(\vec{r})dr=0\ \ j\ge 1. \tag{11}$$

In other words, the operator A_0 maps the fundamental mode eigenfunction in (1) identically to zero and makes the higher mode eigenfunctions in (1) decay by a factor of the ratio of their respective eigenvalue to the fundamental mode eigenvalue. Therefore, the transformation of the system of (6) and (7) to a standard stochastic model may enable one to compute the dominance ratio k_1/k_0 through time series analysis.

Now, we consider the discrete form of (6) and (7) with $\mathrm{O}(N^{-1/2})$ terms ignored and introduce its observation function:

$$\vec{e}^{\,(m)}(\vec{r})=A_0\vec{e}^{\,(m-1)}(\vec{r})+\vec{\varepsilon}^{\,(m)}(\vec{r}), \tag{12}$$

$$E\left[\vec{\varepsilon}^{\,(p)}(\vec{\varepsilon}^{\,(q)})^t\right]=0, \tag{13}$$

$$\vec{y}^{\,(m)}=C\vec{e}^{\,(m)}, \tag{14}$$

where $\vec{e}^{\,(m)}$ and $\vec{\varepsilon}^{\,(m)}$ are $p\times 1$ matrices, A_0 is assumed to be the operator in (8) for functional cases and the corresponding $p\times p$ matrix for discrete cases, and C is an observation matrix with p columns. The addition of a linear observation function (14) is a new approach compared to previous work on discrete models [2, 3], which enables one to apply Akaike's theory of Markovian representation of stochastic processes [4] to derive an ARMA representation of the system of Eqs. (12) and (14). To proceed further, the characteristic polynomial of the matrix A_0 is introduced:

$$|\,\lambda I-A_0\,|=\lambda^p+\sum_{n=1}^{p}a_n\lambda^{p-n} \tag{15}$$

where λ is scalar and I is the identity matrix. The largest root of (15) is assumed to be the dominance ratio k_1/k_0 by Eqs. (9)-(11). For sufficiently large p, the i^{th} largest root of (15) would give k_i/k_0 The Cayley-Hamilton theorem states that the coefficient a's in (15) satisfy

$$A_0^p+\sum_{n=1}^{p}a_nA_0^{p-n}=0. \tag{16}$$

The system of Eqs. (12) and (14) combined with (16) yields

$$\begin{aligned}&\vec{y}^{\,(n+p)}+a_1\vec{y}^{\,(n+p-1)}+\cdots+a_p\vec{y}^{\,(n)}\\&=C_0\vec{\varepsilon}^{\,(n+p)}+C_1\vec{\varepsilon}^{\,(n+p-1)}+\cdots+C_{p-1}\vec{\varepsilon}^{\,(n+1)},\end{aligned} \tag{17}$$

where matrices C_i are defined as

$$C_i=C\left(A_0^i+a_1A_0^{i-1}+\cdots+a_iI\right),\ C_0=C \tag{18}$$

Eq. (17) is a multivariate ARMA process of order p and p-1. However, when the observation matrix C is $1\times p$ row vector, the observation $\vec{y}$ becomes scalar and the right hand of Eq. (17) is also scalar. In this case, one can easily perform time series analysis of Eq. (17), since many numerical and statistical libraries have routines for scalar ARMA models and/or the nonlinear least square routines to compute these coefficients. In addition, Eq. (17) with Eq. (13) is a general statistical model that can be applied to any criticality problem unlike a previous model specific to two fissile component systems [5]. When the observation matrix C has unity for one component and zero otherwise, the observation $\vec{y}$ becomes the source at the bin corresponding to the unity component. Thus, one can compute the coefficients a's through the ARMA fitting of the source, and the largest root of the characteristic polynomial yields the dominance ratio k_1/k_0. In the next section, we compute the dominance ratio through binary source bins (p=2).

NUMERICAL RESULTS

We compute the dominance ratio of two-dimensional homogeneous squares of various sizes with isotropic and energy-independent cross sections; $\Sigma_t = 1.0\ cm^{-1}$, $\Sigma_a = 0.3\ cm^{-1}$, and $\nu\Sigma_f = 0.24\ cm^{-1}$. The reference values of the dominance ratio are obtained by analyzing the spectral radius of the outer iterations in a discontinuous finite element discrete ordinate computation [6]. For the ARMA fitting of the source, we utilize a time series analysis routine in the IMSL statistical library [7], which is based on a standard nonlinear least square algorithm [8]. The largest root of the characteristic polynomial is the MC estimation of dominance ratio. Its statistical error is evaluated by the error propagation formula using the covariance matrix of the coefficient *a*'s. For quality assurance purposes, a stationarity check is performed for each MC result using relative entropy [1]. As shown in Fig. 1, Monte Carlo computations agree very well with deterministic computations.

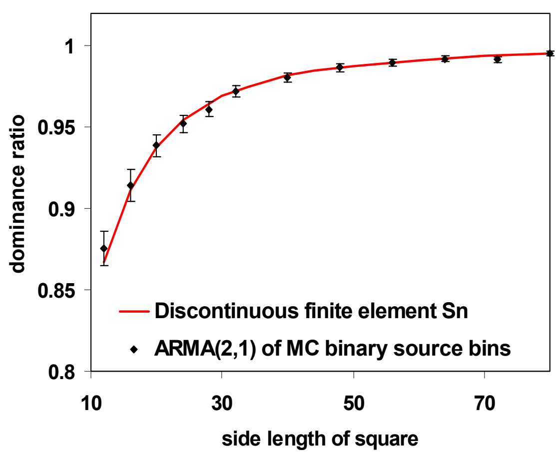

Fig. 1. Dominance ratio of 2D homogeneous square problems of various sizes (error bars showing 95% confidence interval; 40000 histories per cycle and 20000 active cycles)

REFERENCES

1. T.Ueki, F.B. Brown, D.K. Parsons and D.E. Kornreich, "Autocorrelation and Dominance Ratio in Monte Carlo Criticality Calculations," Nucl. Sci. Eng. submitted.
2. R.J. Brissenden and A.R. Garlick, "Biases in the estimation of Keff and its error by Monte Carlo methods," Annals of Nuclear Energy, **13**, 2, 63 (1986).
3. E.M. Gelbard and A.G. Gu, "Biases in Monte Carlo eigenvalue calculations," Nucl. Sci. Eng., **117**, 1 (1994).
4. H. Akaike, "Markovian representation of stochastic processes and its application to the analysis of autoregressive moving average processes," Annals of the Institute of Statistical Mathematics, **26**, 363 (1974).
5. T. Yamamoto, T. Nakamura and Y. Miyoshi, "Fission source convergence of Monte Carlo criticality calculations in weakly coupled fissile arrays," Journal of Nuclear Science and Technology, **37**, 41 (2000).
6. T.A. Wareing, J.M. McGhee, J.E. Morel and S.D. Pautz, "Discontinuous finite element S_N methods on three-dimensional unstructured grids," Nucl. Sci. Eng., **138**, 256 (2001).
7. IMSL Stat/Library Volume 2, Visual Numerics, Inc., Houston TX (1997).
8. G.E.P. Box, G.M. Jenkins and G.C. Reinsel, Time series analysis: forecasting and control, 3rd ed. Prentice-Hall, Inc., Upper Saddle River, NJ (1994).