Monte Carlo Alpha Iteration Algorithm for a Subcritical System

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1. Introduction

The prompt neutron decay constant (referred to as α) is a basic neutronic parameter which can be directly measured in the reactor physics test. In the Monte Carlo (MC) neutron transport calculations, *k*-iteration-based methods with considering 'time absorption' or 'time production' [1-5] have been used for the α-mode eigenvalue calculations. However these traditional methods are observed to cause instability for highly subcritical systems which leads to abnormal terminations from a sudden increase of the time sources [4,5]. In this paper, we propose a stable α calculation algorithm in which the population of the time sources is controlled by the power method for the time source. The effectiveness of the new α iteration method is examined for two-group infinite homogeneous problems and the Godiva problem [6].

2. Derivation of α Iteration algorithm

The α-mode eigenvalue equation for prompt neutron can be expressed in operator notation as

$$\mathbf{T}\Phi = \mathbf{F}\Phi + S_t; \tag{1}$$

$$\mathbf{T}\Phi = \mathbf{\Omega}\cdot\nabla\Phi(\mathbf{r},E,\mathbf{\Omega}) + \Sigma_t(\mathbf{r},E)\Phi(\mathbf{r},E,\mathbf{\Omega}) - \int_{E'}dE'\int_{4\pi}d\mathbf{\Omega}'\Sigma_s(\mathbf{r},E'\to E,\mathbf{\Omega}'\to\mathbf{\Omega})\Phi(\mathbf{r},E',\mathbf{\Omega}'), \tag{2}$$

$$\mathbf{F}\Phi = \frac{\chi_p(E)}{4\pi}\int_{E'}dE'\int_{4\pi}d\mathbf{\Omega}'\nu_p(E')\Sigma_f(\mathbf{r},E')\Phi(\mathbf{r},E',\mathbf{\Omega}'), \tag{3}$$

$$S_t = \alpha v(E)^{-1}\Phi(\mathbf{r},E,\mathbf{\Omega}), \tag{4}$$

where Φ is the neutron angular flux and v is a neutron speed. Other notations follow convention.

Treating the time source S_t as an external source, one can transform Eq. (1) for Φ into an integral equation for the collision density ψ defined by $\Sigma_t\Phi$ as

$$\psi(\mathbf{r},E,\mathbf{\Omega}) = \int d\mathbf{r}'T(\mathbf{r}'\to\mathbf{r}\mid E,\mathbf{\Omega})S_t(\mathbf{r}',E,\mathbf{\Omega}) + \int d\mathbf{r}'\int_{E'}dE'\int_{4\pi}d\mathbf{\Omega}'K(\mathbf{r}',E',\mathbf{\Omega}'\to\mathbf{r},E,\mathbf{\Omega})\psi(\mathbf{r}',E',\mathbf{\Omega}'); \tag{5}$$

$$K(\mathbf{r}',E',\mathbf{\Omega}'\to\mathbf{r},E,\mathbf{\Omega}) = T(\mathbf{r}'\to\mathbf{r}\mid E,\mathbf{\Omega})\cdot C(E',\mathbf{\Omega}'\to E,\mathbf{\Omega}\mid\mathbf{r}'), \tag{6}$$

$$C(E',\mathbf{\Omega}'\to E,\mathbf{\Omega}\mid\mathbf{r}') = \sum_r\frac{\nu_r\Sigma_r(\mathbf{r}',E')}{\Sigma_t(\mathbf{r}',E')}f_r(E',\mathbf{\Omega}'\to E,\mathbf{\Omega}), \tag{7}$$

$$T(\mathbf{r}'\to\mathbf{r}\mid E,\mathbf{\Omega}) = \frac{\Sigma_t(\mathbf{r},E)}{|\mathbf{r}-\mathbf{r}'|^2}\exp\left[-\int_0^{|\mathbf{r}-\mathbf{r}'|}\Sigma_t\left(\mathbf{r}-s\frac{\mathbf{r}-\mathbf{r}'}{|\mathbf{r}-\mathbf{r}'|},E\right)ds\right]\delta\left(\mathbf{\Omega}\cdot\frac{\mathbf{r}-\mathbf{r}'}{|\mathbf{r}-\mathbf{r}'|}-1\right), \tag{8}$$

where ν_r is the average number of neutrons produced from a reaction type *r* and $f_r(E',\mathbf{\Omega}'\to E,\mathbf{\Omega})dEd\mathbf{\Omega}$ the probability that a collision of type *r* by a neutron of direction $\mathbf{\Omega}'$ and energy E' will produce a neutron in direction interval $d\mathbf{\Omega}$ about $\mathbf{\Omega}$ with energy in dE about E.

Then the Neumann series solution to Eq. (5) can be expressed as

$$\psi(\mathbf{r},E,\mathbf{\Omega}) = \sum_{j=0}^{\infty}\int d\mathbf{r}'\int dE_0\int d\mathbf{\Omega}_0K_j(\mathbf{r}',E_0,\mathbf{\Omega}_0\to\mathbf{r},E,\mathbf{\Omega}) \times\int d\mathbf{r}_0T(E_0,\mathbf{\Omega}_0;\mathbf{r}_0\to\mathbf{r}')S_t(\mathbf{r}_0,E_0,\mathbf{\Omega}_0); \tag{9}$$

$$K_j(\mathbf{r}',E_0,\mathbf{\Omega}_0\to\mathbf{r},E,\mathbf{\Omega}) = \int d\mathbf{r}_1\int dE_1\int d\mathbf{\Omega}_1\cdots\int d\mathbf{r}_{j-1}\int dE_{j-1}\int d\mathbf{\Omega}_{j-1} \times K(\mathbf{r}_{j-1},E_{j-1},\mathbf{\Omega}_{j-1}\to\mathbf{r},E,\mathbf{\Omega})\cdots K(\mathbf{r}',E_0,\mathbf{\Omega}_0\to\mathbf{r}_1,E_1,\mathbf{\Omega}_1). \tag{10}$$

Multiplying $\alpha v^{-1}\Sigma_t^{-1}$ on both sides of Eq. (9), one can obtain the α-mode eigenvalue equation for the time source as

$$S_t = \alpha\mathbf{R}S_t; \tag{11}$$

$$\mathbf{R}S_t = \frac{1}{v\Sigma_t(\mathbf{r},E)}\sum_{j=0}^{\infty}\int d\mathbf{r}'\int dE_0\int d\mathbf{\Omega}_0K_j(\mathbf{r}',E_0,\mathbf{\Omega}_0\to\mathbf{r},E,\mathbf{\Omega}) \times\int d\mathbf{r}_0T(E_0,\mathbf{\Omega}_0;\mathbf{r}_0\to\mathbf{r}')S_t(\mathbf{r}_0,E_0,\mathbf{\Omega}_0); \tag{12}$$

The fundamental mode solution to Eq. (11) can be found by means of the power method:

$$S_t^i = \alpha^i\mathbf{R}S_t^{i-1}, \tag{13}$$

$$\alpha^i = 1\Big/\int d\mathbf{r}\int dE\int d\mathbf{\Omega}\ \mathbf{R}S_t^{i-1}, \tag{14}$$

where *i* is the iteration index.

Whenever a collision occurs in the course of the power iteration governed by Eq. (13), the source neutrons for the next iteration (*i*+1) are sampled as many as

$$M_{ijk} = \left[\frac{\alpha^{i-1}}{v(\mathbf{r}_{ijk},E_{ijk})\Sigma_t(\mathbf{r}_{ijk},E_{ijk})} + \xi\right], \tag{15}$$

where *j* and *k* are indices of time source and collision, respectively. [*x*] denotes the largest integer not exceeding *x*. ξ is a uniform random number on the interval of (0,1]. Note that location, energy, and direction of these sources are $(\mathbf{r}_{ijk},E_{ijk},\mathbf{\Omega}_{ijk})$ and that α^{i-1} in Eq. (15) plays a role of controlling the total number

of time sources per iteration. The weight of the time sources of iteration i, w_i, is set to

$$w_i = \frac{M}{M_i};\ M_i = \sum_j \sum_k M_{ijk}\,, \tag{16}$$

where M is a number of sources per iteration initially set by a code user. Eq. (14) implies that α^i can be estimated by the collision estimator as

$$\overline{\alpha^i} = \frac{M}{\sum_j \sum_k v(\mathbf{r}_{ijk}, E_{ijk})^{-1} \Sigma_t(\mathbf{r}_{ijk}, E_{ijk})^{-1}}\,. \tag{17}$$

3. Numerical Results

The new α iteration algorithm and the conventional iteration method [5] have been implemented in McCARD [7] and tested for two-group infinite homogeneous medium problems and Godiva.

3.1 Two-group infinite homogeneous problems

Table I shows two-group cross sections varying the prompt criticality k_p. The differential scattering cross section of the first group, Σ_{s21}, is set to 0.265714, 0.197143, 0.128571, 0.060000, or 0.008571, which correspond to k_p of 0.9, 0.7, 0.5, 0.3, or 0.15.

Table I: Two-group cross sections for infinite homogeneous problems

Cross section	First Gr. (g=1)	Second Gr. (g=2)
Σ_t	0.50	0.50
Σ_f	0.025	0.175
ν	2.0	2.0
Σ_{sgg}	0.10	0.20
$\Sigma_{sg'g}$ ($g \neq g'$)	variable	0.00
χ_p	1.0	0.0
$1/v$ [sec/cm]	2.28626×10^{-10}	1.29329×10^{-6}

The MC α calculations are performed for 1000 active iterations on 10,000 sources per iteration. Table II shows comparisons of α's calculated by the new algorithm and the conventional method with analytic solutions. From the table, one can see that the MC results from the new method agree well with the analytic references within 95% confidence intervals while the conventional method fails when k_p are 0.3 and 0.15.

Table II: α comparisons for infinite homogeneous problems

k_p	Ref. α	Conventional method (SD)	New method (SD)
0.90	26507.1	26500.1 (12.8)	26524.4 (14.0)
0.70	79523.4	79574.6 (33.8)	79522.6 (18.1)
0.50	132544.0	132518.0 (70.8)	132539.0 (20.9)
0.30	185568.0	fail	185554.0 (26.6)
0.15	225338.0	fail	225328.0 (31.3)

As observed in Table II, the traditional iteration method in which the time sources are generated at all the collision sites with probability of $\alpha/(v\Sigma_t)$ in a neutron history suffers from abnormal terminations. In order to investigate these abnormal terminations, we introduce an expected number of time sources per source neutron.

For simplicity, suppose a one-group infinite homogeneous problem written as

$$\Sigma_r \phi = \nu\Sigma_f \phi + \frac{\alpha}{v}\phi\,, \tag{18}$$

with α of $v(\Sigma_r - \nu\Sigma_f)$.

In the MC simulations of Eq. (18), the production probability of the time source p_α and the neutron absorption probability p_{abs} become

$$p_\alpha = \frac{\alpha / v}{\Sigma_t}\,, \tag{19}$$

$$p_{abs} = \frac{\Sigma_r}{\Sigma_t}\,. \tag{20}$$

Then the expected number of time sources per source neutron, N_{time} can be written by

$$\begin{aligned} N_{time} &= p_\alpha + (1-p_{abs})\,p_\alpha + (1-p_{abs})^2\,p_\alpha + \cdots \\ &= \frac{p_\alpha}{1-(1-p_{abs})} = \frac{\alpha/v}{\Sigma_t}\frac{\Sigma_t}{\Sigma_r} = \frac{\alpha}{v\Sigma_r}. \end{aligned} \tag{21}$$

When N_{time} becomes greater than 1, the expectation of the total number of time sources in a single history becomes infinity which leads to the abnormal termination. Therefore the upper limit of α that assures the stability of the MC calculations can be expressed from Eq. (21) as

$$\alpha < v\Sigma_r. \tag{22}$$

By inserting the analytic value of α of $v(\Sigma_r - \nu\Sigma_f)$ into Eq. (22), we can find that the condition of Eq. (22) is satisfied for the one-group infinite homogeneous problem.

However, abnormal terminations are able to occur in the conventional method in which α is updated by

$$\alpha^{i+1} = \alpha^i / k^i \tag{23}$$

where i is the iteration index and k is the multiplication factor. Because of this procedure that α is divided by k, a statistical uncertainty of k causes large fluctuations of α, and therefore the condition of Eq. (22) may not be satisfied.

In the case of two-group problem, the approximate upper limit of α can be obtained from the thermal group because Eq. (22) shows the upper limit of α is proportional to the neutron speed.

In the case of k_p of 0.3, the upper limit of α, α_{limit} can be obtained

$$\alpha_{\text{limit}} = v_2\Sigma_{r2} = 2.3196\times10^5. \quad (24)$$

The ratio of the upper limit to the reference α is about 1.25. Figure 1 shows α^j for k_p of 0.3 with 10^5 and 10^7 histories per cycle. From the figure, we can observed that the abnormal terminations happen at 6-th cycle by α^j=241187.0 for the 10^5 history case and 8-th cycle by α^j=233344.0 for the 10^7 history case because α^j becomes larger than α_{limit}.

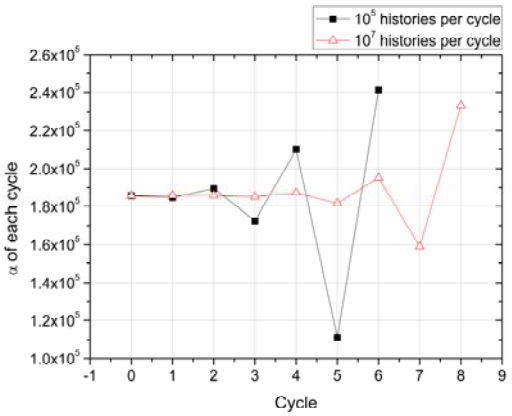

Fig. 1. Fluctuation of α versus cycles

3.2 Godiva problem

The MC α calculations with continuous-energy cross section libraries produced from ENDF/B-VII.0 are conducted for Godiva [6]. The McCARD α calculations are performed for 1000 active iterations on 10,000 sources per iteration. Table III shows a comparison of the McCARD result with α from an exponential fit of a numerical pulsed neutron experiment.

Table III: α estimation for Godiva

	Ref. (Err.[%])	McCARD (RSD[%])
Godiva	1.15076×10^6 (0.52)	1.16506×10^6 (0.35)

4. Conclusions

A new MC α calculation method is developed to estimate the fundamental mode α eigenvalue in subcritical systems. In the new α iteration algorithm, the time sources are iteratively updated while the fission sources are updated in the conventional method. It is demonstrated that the new method does not have the instability problem in two-group homogeneous problems with large subcriticality.

REFERENCES

[1] D. Brockway, P. Soran, P. Whalen, "Monte Carlo α calculation," LA-UR-85-1224, Los Alamos National Laboratory, 1985.
[2] D. E. Cullen, "Users Manual for TART 2002: A Coupled Neutron-Photon 3-D, Combinatorial Geometry Time Dependent Monte Carlo Transport Code," UCRL-ID-126455-REV-4, Lawrence Livermore National Laboratory, 2003.
[3] T. Ye, C. Chen, W. Sun, B. Zhang, D. Tian, "Prompt Time Constants of a Reflected Reactor," T. Fukahori (Ed.), Proc. 2006 Symposium on Nuclear Data, Tokai-mura, Ibaraki-ken, Japan, Jan. 25-26, 2007.
[4] T. Yamamoto, "Higher Order α Mode Eigenvalue Calculation by Monte Carlo Power Iteration," *Prog. Nucl. Sci. Technol.*, 2, 826, 2011.
[5] A. Zoia, E. Brun, F. Malvagi, "Alpha Eigenvalue Calculations with TRIPOLI-4," *Ann. Nucl. Energy*, 63, 274, 2014.
[6] J. Blair Briggs (ed.), "International Handbook of Evaluated Criticality Safety Benchmark Experiments," NEA/NSC/DOC(95)03/I, Nuclear Energy Agency, Paris, 2004.
[7] H. J. Shim, et al., "McCARD: Monte Carlo Code for Advanced Reactor Design and Analysis," *Nucl. Eng. Technol.*, 44[2], 161, 2012.