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Implementation of the modified power iteration method to two-group Monte Carlo eigenvalue problems

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ABSTRACT

In nuclear engineering field, the Monte Carlo method has been used to solve the eigenvalue or criticality problem for many years. The theoretical basis for solving the eigenvalue problem is the power iteration method, which exhibits slow convergence when the dominance ratio of the system is close to one. To overcome this drawback, a modified power iteration method, which could compute the first two eigenpairs at the same time, was proposed and its validity was exemplified for one-dimensional mono-energetic problems. In this paper, we implemented this method to one-dimensional two-group problems and proved its validity for these problems. This work indicates the capability of the modified power iteration method to solve practical multi-group or continuous energy problems.

1. Introduction

The most frequently applied principle of using the Monte Carlo method to solve nuclear criticality or eigenvalue problems is the same as in deterministic methods, i.e., power iteration method (Golub and Van Loan, 1996). The convergence rate of the power iteration method depends on the dominance ratio of the operator or matrix, which challenges the Monte Carlo method when the problem has a high dominance ratio close to one. A high dominance ratio generally requires the Monte Carlo method to simulate the problem for a very long time before the fission source distribution converges; moreover, this initial portion of the simulation has to be discarded from tallying. Therefore, convergence acceleration methods are desired to reduce the uncertainty of the results with significantly less computational cost. Recently, a new means to accelerate the fission source convergence was proposed by Booth and Gubernatis (2009) using a modified power iteration method. In addition to the capability of convergence acceleration, the new method can also calculate the second eigenpair simultaneously with the fundamental eigenpair. We confirmed the validity of the method with a one-dimensional mono-energetic problem and explored the behavior of estimated variance (Shi and Petrovic, 2010), but—while in principle expected—no examples or illustrations were available to guarantee that the modified power iteration method will work for a multi-group or continuous energy problem. In this paper, we will examine the capability of the modified power iteration method when applied to one-dimensional problems with two energy groups.

2. Review of the modified power iteration method

We first review some basic properties of eigenfunctions and eigenvalues. An eigenvalue problem is to find the function(s) ψ and value(s) k satisfying equation $A\psi = k\psi$, where A represents an operator or a matrix. There exist certain values k_i, which are called eigenvalues, and functions ψ_i, which are called eigenfunctions, satisfying the relation:

$$A\psi_i = k_i\psi_i, \quad \text{where} \quad |k_1| > |k_2| > |k_3| > \cdots\cdots. \tag{1}$$

The eigenvalue with the largest absolute value k_1 is called the fundamental eigenvalue and the corresponding ψ_1 is called the fundamental eigenfunction. Similarly, the eigenvalue with the second largest absolute value k_2 is called the second eigenvalue and the pairing eigenfunction ψ_2 is called the second eigenfunction. Generally, a well-behaved function ψ can be decomposed over the basis of all the eigenfunctions. By repeatedly left-multiplying A with certain renormalization, the well-behaved initial function ψ will converge to the fundamental eigenfunction:

$$\lim_{n\to\infty} \frac{1}{k_1^n} A^n \psi = \psi_1. \tag{2}$$

One could also estimate the fundamental eigenvalue k_1:

$$k_1 = \lim_{n\to\infty} \frac{A^n\psi}{A^{n-1}\psi}. \tag{3}$$

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If a parameter or unknown x is introduced as a coefficient of the decomposition of a well-behaved function ψ (Booth, 2006), we may write:

$$\psi = \sum_i (a_i + b_i x)\psi_i, \tag{4}$$

where a_i and b_i are general coefficients.

Similar estimates of the eigenfunction and eigenvalue with renormalization will become:

$$\lim_{n\to\infty} \frac{1}{k_1^n} A^n \psi = \lim_{n\to\infty} \frac{1}{k_1^n}((a_1 + b_1 x)k_1^n \psi_1 + (a_2 + b_2 x)k_2^n \psi_2), \tag{5}$$

$$\lim_{n\to\infty} \frac{A^n \psi}{A^{n-1}\psi} = \lim_{n\to\infty} \frac{(a_1 + b_1 x)k_1^n \psi_1 + (a_2 + b_2 x)k_2^n \psi_2}{(a_1 + b_1 x)k_1^{n-1} \psi_1 + (a_2 + b_2 x)k_2^{n-1} \psi_2}. \tag{6}$$

According to Eq. (6), an estimate of the eigenvalue with unknown x can be performed in two different sub-regions of the system. The convergence condition requires that the two estimates are equal, so by equating the two estimates, a quadratic equation in x is obtained. These two roots, when inserted into Eq. (6), produce the fundamental eigenvalue k_1 and the second eigenvalue k_2, respectively. The corresponding eigenfunctions are also obtainable by inserting x into Eq. (5). One advantage of this method is the potential to increase the convergence rate from k_2/k_1 to k_3/k_1. Thus, if the difference of these two ratios is significant, the reduction of the required computational time may be dramatic.

However, as the convergence goes on, the difference between the coefficients, $\{a_i\}$ and $\{b_i\}$, will diminish and the modified power iteration method will numerically collapse (i.e., be able to generate only the first eigenpair). Several refinements (Gubernatis and Booth, 2008; Shi and Petrovic, 2010) have been proposed to update the function ψ to avoid the collapse. These refinements enabled the modified power iteration method to simulate the problem as long as required to reduce the statistical uncertainty caused by the Monte Carlo method to the desired level.

3. Monte Carlo simulation procedure

We implemented the modified power iteration method to eigenvalue problems with two energy groups and examined the validity of obtained results. For simplicity, we only used the collision estimator to estimate k_{eff}. The simulation procedure is essentially the same as that for a mono-energetic problem: we first divided the entire system into two sub-regions; then, we generated two sets of sources with different distributions to initialize the simulation; we estimated the k_{eff} in each sub-region with a parameter x multiplying one of the estimates by the Monte Carlo simulation; finally, we solved the quadratic equation for x to compute the fundamental and second eigenpair, and generated two source distributions again for the next generation, which is based on the second refinement in Gubernatis and Booth (2008).

This scheme requires weight cancellation of the fission source distributions, which is hard to perform because the source distribution only includes the positions of fission events. Several weight cancellation and source generating approaches are available in the references (Booth, 2003; Booth and Gubernatis, 2009; Yamamoto, 2009; Booth and Gubernatis, 2010). In this work, we apply the method presented in Yamamoto's work (2009), which projects the source distribution to tally meshes. The general cell-based flux tally with collision estimator for a single material with one energy group is given by the following equation:

$$\text{Cell flux} = \frac{1}{V * N} * \sum_i \frac{w_i}{\Sigma_t}, \tag{7}$$

where V is the mesh volume; N is the total number of particles used; i is the collision index taking place in the specific mesh; w_i is the weight of particles; and Σ_t is the total cross-section for each collision.

However, the cell flux tally has some disadvantages, which make it impractical in multi-group simulations with non-fissionable materials. Therefore, we selected to use the total fission density distribution to represent the spatial convergence of the problem. The fission density tally with collision estimator for a single material is shown in the following equation:

$$\text{Fission density} = \frac{1}{V * N} * \sum_i \frac{w_i * \bar{\nu} * \Sigma_f}{\Sigma_t}. \tag{8}$$

This is an energy-integrated tally that is reasonable to use in reactor physics since the fission source spectrum at each location should be almost iteration independent. As a result, it is easily applicable for either multi-group problems or continuous energy problems. Therefore, by employing tally meshes small enough so that the approximation is accurate enough, the weight cancellation may be performed on the mesh basis.

After the weight cancellation with the fission density tally, we generated the same number of particles in each tally mesh with specific weights adjusted to conserve the total source weight in each generation. In addition to the fission density tally, we still recorded the cell flux tally to compute the eigenfunctions.

4. Problem one: single-region problem

The first problem we would like to simulate is a one-dimensional two-group problem with single fission material, whose postulated cross-section data are listed in Table 1. The cross-section values chosen here are not necessarily realistic, but our purpose is to verify the validity of the modified power iteration method and our implementation. The system extends from −4.5 cm to 4.5 cm along the Z direction with vacuum on either side. We divided the system into two sub-regions, the left one (−4.5–0 cm) and the right one (0–4.5 cm), to estimate the k_{eff} separately. We also divided the system into 100 meshed evenly along the Z direction for the flux estimate and fission density computation.

We used the MCNP5 (X-5 Monte Carlo Team, 2003) with user-specified multi-group cross-section data to generate reference results. The reference simulation employed 50,000 particles per generation for 1000 active generations after the convergence of the fission source. Our computation with the modified power iteration employed 10,000 particles per generation, 50 inactive generations, and 100 active generations. Table 2 compares the k_{eff} results from MCNP5 and our computation. This comparison of the

Table 1
Two-group data for fission material (cross-section in cm^{-1}).

Σ_t	Σ_c	Σ_f	ν	$\Sigma_{\text{in-group}}$	$\Sigma_{\text{out-group}}$	
Group 1						
1.0	0.05	0.05	3.0	0.1	0.8	1.0
Group 2						
1.0	0.2	0.1	3.0	0.0	0.7	0.0

Table 2
Comparison of k_{eff} for problem one.

MCNP5	Modified method	Difference
0.94386 ± 0.00008	0.94401 ± 0.00019	0.7σ