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A New Accumulation Scheme for the Monte Carlo Implementation of the Modified Power Method

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Abstract – *The Modified Power Method (MPM) has been implemented and applied to three-dimensional (3D) criticality eigenvalue problems. Monte Carlo (MC) implementation of the MPM has been difficult due to the inherent statistical noises introduced during the MC simulations. The one-cycle tally should be avoided because it contains too much noises and cause big fluctuation in the MPM simulation. Therefore, accumulation should be adopted. In addition, previous studies have shown that to obtain the first several eigenmodes for the multi-dimensional problems, more number of sub-regions than the number of desired eigenmodes should be adopted for the calculation of the transfer matrix, which makes the linear system of equations become over-determined and the accumulation become problematic. In this paper, a proper accumulation scheme was developed, which was based on the preprocessing of the neutron weight integrals. The performance of the proposed method has been successfully demonstrated with the 3D numerical tests.*

I. INTRODUCTION

In this work, the modified power method (MPM) [1-7] has been applied to 3D criticality eigenvalue problems to demonstrate its performance, and discussions on the implementation issues are presented. A new Monte Carlo accumulation scheme for the MPM will be proposed.

Previous study has shown that the application of MPM to 2D/3D problems may be unstable due to the degeneracy issues [8]. The way to solve this problem is to use more number of sub-regions (coarse meshes) than the number of desired eigenmodes to distinguish the first several eigenmodes. In this case, the solving of the transfer matrix (TM) may have some problems. These issues will be explained and will be followed by the proposed methods to solve the issues and the discussion on 3D applications.

II. IMPLEMENTATION OF MPM FOR 3D APPLICATIONS

1. Review of the MPM

The *N* initial distributions and the results after applying the power operator are:

$$\begin{aligned} \psi_j &= \sum_{i=1}^{N} c_{ij}\phi_i,\ j=1,...,N, \\ A\psi_j &= \sum_{i=1}^{N} c_{ij}k_i\phi_i,\ j=1,...,N, \end{aligned} \tag{1}$$

where (k_i, ϕ_i) are the eigenpairs of the system, ψ_j is the *j*-th distribution, *A* is the power operator and the higher modes of order larger than *N* are neglected.

The first *N* eigenfunctions can be solved by the linear combination of the *N* distributions:

$$\begin{pmatrix} \psi_1 & \cdots & \psi_N \end{pmatrix} \begin{pmatrix} x_{11} & \cdots & x_{1N} \\ \vdots & \ddots & \vdots \\ x_{N1} & \cdots & x_{NN} \end{pmatrix} = \begin{pmatrix} \phi_1 & \cdots & \phi_N \end{pmatrix}. \tag{2}$$

For any sub-region R_j of the system, the power operator and eigenfunctions satisfy:

$$\int_{R_j} A\phi_i dr = k_i \int_{R_j} \phi_i dr. \tag{3}$$

Dividing the whole system into N sub-regions, denoting $W_{ij} = \int_{Rj} A\psi_i dr$, $V_{ij} = \int_{Rj} \psi_i dr$ and $Q_{ij} = \int_{Rj} \phi_i dr$, and according to Eqs. (1), (2) and (3), there is:

$$\begin{pmatrix} W_{11} & \cdots & W_{1N} \\ \vdots & \ddots & \vdots \\ W_{N1} & \cdots & W_{NN} \end{pmatrix} \begin{pmatrix} x_{11} & \cdots & x_{1N} \\ \vdots & \ddots & \vdots \\ x_{N1} & \cdots & x_{NN} \end{pmatrix} = \begin{pmatrix} V_{11} & \cdots & V_{1N} \\ \vdots & \ddots & \vdots \\ V_{N1} & \cdots & V_{NN} \end{pmatrix} \begin{pmatrix} x_{11} & \cdots & x_{1N} \\ \vdots & \ddots & \vdots \\ x_{N1} & \cdots & x_{NN} \end{pmatrix} \begin{pmatrix} k_1 & \cdots & 0 \\ \vdots & \ddots & \vdots \\ 0 & \cdots & k_N \end{pmatrix}, \tag{4}$$

and

$$\begin{pmatrix} V_{11} & \cdots & V_{1N} \\ \vdots & \ddots & \vdots \\ V_{N1} & \cdots & V_{NN} \end{pmatrix} \begin{pmatrix} x_{11} & \cdots & x_{1N} \\ \vdots & \ddots & \vdots \\ x_{N1} & \cdots & x_{NN} \end{pmatrix} = \begin{pmatrix} Q_{11} & \cdots & Q_{1N} \\ \vdots & \ddots & \vdots \\ Q_{N1} & \cdots & Q_{NN} \end{pmatrix}. \quad (5)$$

The eqs. (4) and (5) can be rewritten as:

$$\mathbf{WX = VXK}, \quad (6)$$

and

$$\mathbf{VX = Q}. \quad (7)$$

The TM is defined as:

$$\mathbf{P} = \mathbf{QKQ}^{-1}, \quad (8)$$

where **K** and **Q** consist of the eigenvalues and eigenvectors of the TM. The eigenvalues are of the TM are also the eigenvalues of the system, while the eigenvectors of the TM depend on the sub-region definition. According to Eqs. (6), (7) and (8), there is:

$$\begin{aligned} \mathbf{W} &= \mathbf{VXKX^{-1}} = \left(\mathbf{VX}\right)\mathbf{K}\left(\mathbf{VX}\right)^{-1}\mathbf{V} \\ &= \mathbf{QKQ^{-1}V} = \mathbf{PV}, \end{aligned} \quad (9)$$

so the TM can be solved with

$$\mathbf{P = WV}^{-1}, \quad (10)$$

and then its eigenvectors can be used to solve the linear combination coefficients:

$$\mathbf{X = V^{-1}Q}, \quad (11)$$

which will then be used to update the first *N* eigenfunctions.

2. Extension of the MPM for Multi-Dimensional Problems

Based on last section, the remaining problem for the MPM is how to get the unique *N* sub-regions of the system. For simple 1D homogeneous problems, the system can be divided into *N* uniform meshes. However, for 2D/3D problems, it may be difficult and not practical to find the unique *N* sub-regions.

In previous study, it is proposed to use more number of meshes than the number of modes. In this case, Eq. (6) will become an over-determined equation system. Some techniques need to be developed to solve it.

A. Approach 1

One approach is to rewrite Eq. (6) as:

$$\mathbf{VY} = \mathbf{W}, \quad (12)$$

where

$$\mathbf{Y} = \mathbf{XKX}^{-1}. \quad (13)$$

The solution strategy is: first solve **Y** with least square method based on Eq. (12), and then apply eigen-decomposition to **Y** to get **X** and **K**.

This approach is well suitable for deterministic calculations. For Monte Carlo implementation, this can be done with just one-cycle tally. However, in practice the one-cycle tallies are never used due to the inherent statistical noises.

B. Approach 2

Another approach is to calculate the TM by solving a minimum norm problem:

$$\mathbf{W} = \mathbf{PV}, \quad (14)$$

where $\mathbf{W}, \mathbf{V} \in \mathbf{R}_{M\times N}$, $\mathbf{P} \in \mathbf{R}_{M\times M}$, *M* is the number of sub-regions, $M > N$. Then the eigen-decomposition of the TM is done similarly as Eq. (8), and the first *N* eigenvectors of the TM are used to calculate the **X** matrix:

$$\mathbf{VX} = \mathbf{Q}\left(:, 1:N\right), \quad (15)$$

where $\mathbf{V}, \mathbf{Q} \in \mathbf{R}_{M\times N}$, $\mathbf{X} \in \mathbf{R}_{N\times N}$. **X** can be solved using the least square method. In order to reduce the affection of the stochastic noises, the neutron sources or the TM can be accumulated.

Accumulating the neutron sources works well if there are no degenerated eigenmodes, otherwise it may have problem, because the eigenvectors of the degenerated modes cannot be fixed and will change gradually due to the stochastic noises.

Accumulating the TM does not have the problem of the gradually changing eigenvectors of the degenerated modes. However, another problem arises that the TM calculated with one-cycle tallies have *N* nonzero eigenvalues, while the accumulated TM will have more than *N* nonzero eigenvalues. Fig. 1 shows an example that the first 60 eigenmodes of the BEAVRS 3D whole core model are calculated with MPM, and the accumulated TM can give the first 50 eigenvalues consistently while the rest 10 eigenvalues fluctuate a lot during the simulation.

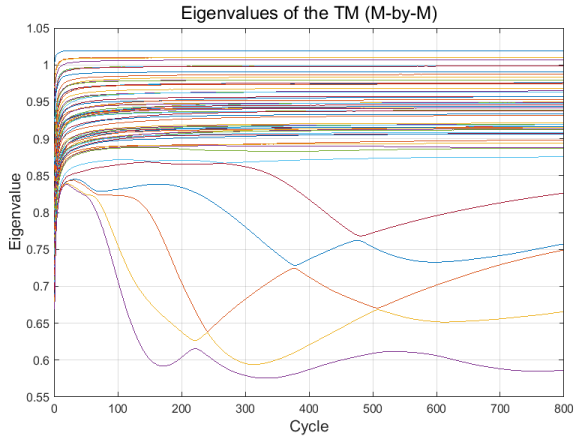

Fig. 1. The first 60 eigenvalues of the TM for a BEAVRS 3D whole core model with 6x6x6 coarse mesh space discretization.

3. The Preprocessing Approach

The problem described previously mainly lies in the mismatch of the number of coarse meshes and the number of modes to be solved. A natural idea is to apply preprocessing to the weight integrals, which is intuitively like mapping the *M* coarse meshes to the specific *N* meshes, so the equation system described by Eq. (6) can be well determined.

Multiplying Eq. (6) with a matrix $\mathbf{G} \in \mathbf{R}_{N\times M}$ from left results in:

$$(\mathbf{GW})\mathbf{X} = (\mathbf{GV})\mathbf{XK}, \tag{16}$$

where $\mathbf{W},\mathbf{V} \in \mathbf{R}_{M\times N}$, $(\mathbf{GW}),(\mathbf{GV}),\mathbf{X},\mathbf{K} \in R_{N\times N}$. Then the linear equation system can be solved with the strategy represented by Eqs. (10) and (11).

The requirements for matrix **G** are:

(1) $(\mathbf{GV})$ should be a square matrix of full rank;

(2) **G** should be kept the same during the simulation.

Requirement (1) is easy to understand. The consideration for requirement (2) is that if **G** changes, the mesh mapping will be different, and so the corresponding TM will also be changed, in which case the TM cannot be accumulated.

There are many choices for matrix **G**. Two options for **G** are recommended in this study. One option is to calculate **G** with the following equation:

$$\mathbf{GV} = \mathbf{I}_{N\times N}. \tag{17}$$

Another option is choosing **G** as:

$$\mathbf{G} = \mathbf{V}^T. \tag{18}$$

Both options satisfy requirement (1) and work well. The BEAVRS 3D whole core model is simulated again with applying the preprocessing matrix and the results are shown in Figs. 2 and 3. It can be noticed that the eigenvalues given by the TM are all stable and consistent with the tallied results.

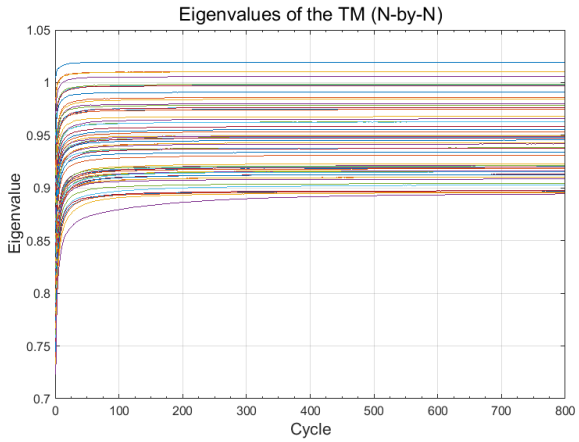

Fig. 2. The first 60 eigenvalues of the TM for the BEAVRS 3D whole core model with preprocess matrix applied.

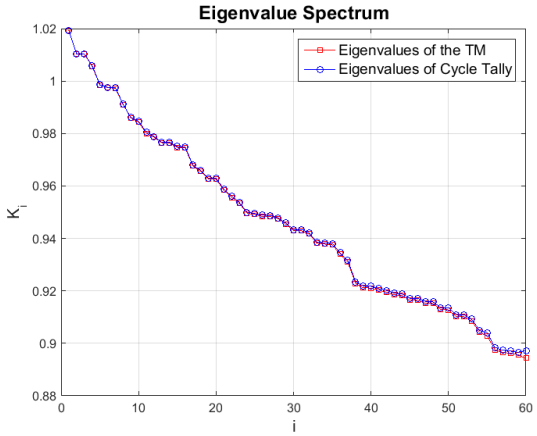

Fig. 3. The eigenvalue spectrum of the BEAVRS 3D whole core model with preprocessing matrix applied.

However, there is another problem related with requirement (2). As previously discussed, if there are degenerated eigenmodes, the corresponding eigenvectors may gradually change cycle by cycle. **G** matrix is determined at the first cycle from which the accumulation begins, so at later cycles it may not work well if the eigenvectors change a lot due to stochastic noises introduced cycle by cycle.

Two measures are recommended to alleviate the problem. One is using better initializations for all the neutron sources; the other is updating the G matrix.

A. Initialization of the Neutron Sources

To start the Monte Carlo simulation, the initial neutron sources are needed. For this study, it is required to distribute the neutron sources over all the active volume, so the neutron source positions are randomly sampled in the entire system space. The neutron weights can be all set to 1.0, or, random numbers, both of which work well.

During the running of the first inactive cycle, the fission matrix (FM) based on the pre-defined coarse meshes is tallied. After finishing the first cycle, the tallied FM is used to calculate the first *N* eigenvectors that are also based on the coarse mesh. The neutron weights for different modes are then corrected with the corresponding eigenvectors. This finishes the initialization process of the MPM.

In case of there are degenerated eigenmodes, after solving the eigenvectors of the FM, all the eigenvectors are corrected to be orthogonal to each other. This can make sure that all the eigenvectors are separated as clearly as possible at the beginning of the simulation, and the inter correlation of the degenerated eigenmodes due to the gradual changing cycle by cycle can be reduced as much as possible.

B. Updating the Preprocessing Matrix

For the later cycles, the eigenvectors of the degenerated eigenmodes may change a lot comparing to their initial values. Updating of the **G** matrix may be needed to ensure the stable performance of the MPM.

Suppose for the previous cycle, the **G** matrix is determined by:

$$\mathbf{G}^{(1)}\mathbf{V}^{(1)} = \mathbf{I}, \tag{19}$$

and the corresponding TM is calculated with:

$$\left(\mathbf{G}^{(1)}\mathbf{W}^{(1)}\right) = \mathbf{P}^{(1)}\left(\mathbf{G}^{(1)}\mathbf{V}^{(1)}\right). \tag{20}$$

For current cycle, the G matrix and the TM are calculated with current cycle tallied values:

$$\begin{aligned} &\mathbf{G}^{(2)}\mathbf{V}^{(2)} = \mathbf{I}, \\ &\left(\mathbf{G}^{(2)}\mathbf{W}^{(2)}\right) = \mathbf{P}^{(2)}\left(\mathbf{G}^{(2)}\mathbf{V}^{(2)}\right). \end{aligned} \tag{21}$$

$\mathbf{P}^{(1)}$ and $\mathbf{P}^{(2)}$ cannot be added together as they are corresponding to different mesh configurations. The relation between $\mathbf{G}^{(2)}$ and $\mathbf{G}^{(1)}$ is:

$$\mathbf{G}^{(2)} = \mathbf{H}\mathbf{G}^{(1)}, \tag{22}$$

and **H** can be calculated with:

$$\mathbf{H}\left(\mathbf{G}^{(1)}\mathbf{V}^{(2)}\right) = \mathbf{I}. \tag{23}$$

Multiplying **H** to both sides of Eq. (13) from left results in:

$$\begin{aligned} \mathbf{H}\mathbf{G}^{(1)}\mathbf{W}^{(1)} &= \mathbf{H}\mathbf{P}^{(1)}\mathbf{G}^{(1)}\mathbf{V}^{(1)} \\ &= \mathbf{H}\mathbf{P}^{(1)}\mathbf{H}^{-1}\mathbf{H}\mathbf{G}^{(1)}\mathbf{V}^{(1)}, \\ \left(\mathbf{G}^{(2)}\mathbf{W}^{(2)}\right) &= \left(\mathbf{H}\mathbf{P}^{(1)}\mathbf{H}^{-1}\right)\left(\mathbf{G}^{(2)}\mathbf{V}^{(2)}\right). \end{aligned} \tag{24}$$

From Eqs. (14) and (17) it can be noticed that $\mathbf{P}^{(2)}$ and $\left(\mathbf{H}\mathbf{P}^{(1)}\mathbf{H}^{-1}\right)$ are corresponding to the same mesh configuration, so they can be accumulated:

$$\mathbf{P} = \left(\mathbf{H}\mathbf{P}^{(1)}\mathbf{H}^{-1}\right) + \mathbf{P}^{(2)}, \tag{25}$$

where $\mathbf{P}$ denotes the accumulated TM up to current cycle.

Therefore, once updating of the preprocessing matrix is required, the **H** matrix is calculated, and then the previously accumulated TM is corrected with this **H** matrix and added with the current cycle TM.

C. Detection of the Degenerated Eigenmodes

Another important issue that should be taken into consideration is the detection of the degenerated eigenmodes.

If degeneracy happens, the eigen-decomposition of the TM cannot give fixed eigenvectors, but rather the linear combinations of its real eigenvectors. In this study, the degeneracy is detected using the eigenvalues of the TM:

$$\left|k_i - k_j\right| < 10^{-3}\,?\quad i, j = 0, \cdots N-1. \tag{26}$$

Once degeneracy is detected, the shape fixing technique described in [9] is used to correct the corresponding eigenvectors.

III. RESULTS

1. The 3D Cube Problem

The multi-group 3D homogeneous cube neutron transport problem is modeled to demonstrate the performance of the MPM. This problem is featured with degeneracy of multiplicity of 3 and 6. The techniques used to deal with degeneracy are very important for the performance.

The 7-group cross sections are from the C5G7 benchmark specification for the 8.7% MOX fuel-clad macroscopic cross sections. The side length of the 3D cube is 400 cm, with black boundary conditions on all the surfaces. The 6x6x6 uniform coarse meshes are used to discretize the system space. The Monte Carlo simulations are done with 100 inactive cycles, 300 active cycles and 500,000 histories per cycle.

The eigenvalue results are shown in Figs. 4-6. The first 32 eigenmodes are calculated at the same time with MPM. It can be confirmed that there is degeneracy of multiplicity of 3 and 6, and the MPM can give consistent results for nearly all the modes. For the last mode, it's not converged completely, since its convergence rate should be determined by k_{32}/k_{31}, which is very close to 1.0.

The Shannon Entropy results are compared and shown in Fig. 7, which confirms the ability of MPM for accelerating the fission source convergence.

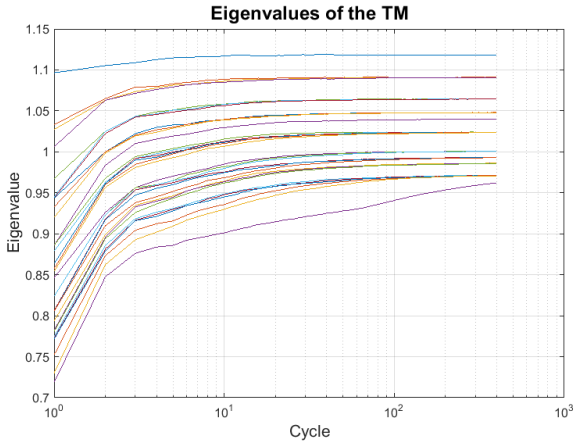

Fig. 4. The eigenvalues of the TM.

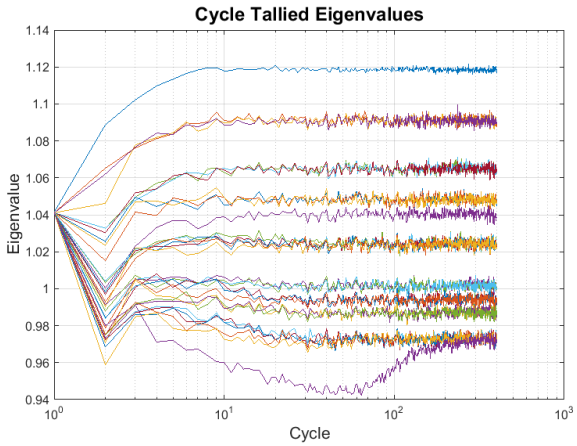

Fig. 5. The cycle tallied eigenvalues (defined as the ratio of the total absolute weight to the number of histories per cycle).

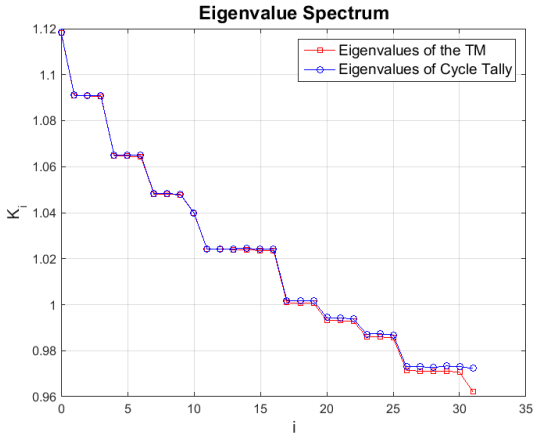

Fig. 6. The eigenvalue spectrum.

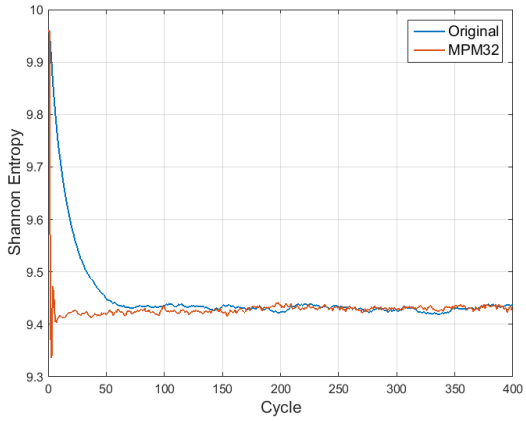

Fig. 7. The Shannon Entropy results.

2. The BEAVRS 3D Whole Core Problem

The 3D PWR core of the BEAVRS benchmark was modeled to demonstrate the capability of the MPM for real practical problems [10]. There was strong geometry heterogeneity, and the continuous energy point cross sections for the materials were used.

The simulation parameters were: 200 inactive cycles / 600 active cycles / 500,000 histories per cycle. The 9x9x9 coarse meshes were used to discretize the whole core space. For the weight cancellation, the 36x36x45 fine mesh configuration was adopted.

For this problem, the results with and without preprocessing are compared. The eigenvalue results without preprocessing are shown in Fig. 1. It is obvious that the last several eigenvalues of the TM fluctuate a lot and are smaller than the normal values. The reason is as following. For every cycle, the current cycle TM of size M-by-M (M=729 for this problem) will be calculated by solving a minimum norm problem while it has only N (N=60 for this problem) nonzero eigenvalues. The corresponding eigenpairs are not the same for the successive two cycles due to the statistical noises, so if the TM of the two cycles are added together,

the accumulated TM may give more than N non-zero eigenvalues, and the last several eigenvalues will usually be smaller than their nominal values.

The results with preprocessing are shown in Figs. 2 and 3. It can be noticed that the performance of the MPM is stable for all the eigenmodes.

IV. CONCLUSIONS

A proper accumulation scheme was developed, aimed at achieving a more stable performance for the MC implementation of the MPM. The new method is based on the preprocessing of the neutron weight integrals, with which the number of elements representing one eigenvector matches well with the number of eigenmodes to be solved. To make it work, the accompanied techniques were developed, including the initialization of the neutron sources and the updating of the preprocess matrix.

The performance of the new method was successfully demonstrated with the 3D cube problem, which features degeneracy of multiplicity of 3 and 6. The techniques dealing the degenerated eigenmodes are very important for this problem. The 3D BEAVRS whole core was also modeled, and the results demonstrate the capability of the MPM for the practical problems.

It is apparent that the MPM can be applied to more general eigenvalue problems. Since the information of the higher modes can be obtained at the same time, there may be a way to reduce the inter-cycle correlation using the higher mode information. This is another topic requiring further investigation.

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