Monte Carlo Higher Modes Calculation based on the Extension of the Noise Propagation Matrix

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Abstract – *The Noise Propagation Matrix Method (NPMM) has been extended to get the higher mode solutions. Previous studies show that the NPMM can be used to compute the dominance ratio (DR) of a system. It is essentially the same as the Coarse Mesh Projection Method (CMPM), both of which use the Noise Propagation Matrix (NPM) to determine the DR, either after finishing the Monte Carlo simulation or on-the-fly during the simulation. Since only the fundamental fission source information is explicitly utilized while the higher mode information is implicitly contained in the statistical noises, the NPMM usually requires thousands of cycles to get an approximated estimation of the DR. In this study, the NPMM is extended by simulating the higher modes explicitly. In this way, smaller number of cycles is required to get an accurate estimation of the DR, and the higher mode solutions can be obtained at the same time with good accuracy and efficiency.*

I. INTRODUCTION

Previous studies show that the Noise Propagation Matrix Method (NPMM) [1], which is essentially the same as the Coarse Mesh Projection Method (CMPM) proposed even earlier [2-8], can be used to compute the dominance ratio (DR) of the system with Monte Carlo simulation. The Noise Propagation Matrix (NPM) is calculated based on a coarse mesh projection of the neutron sources of successive two cycles. The eigenvalues of the NPM corresponding to the system eigenvalue ratios, while the biggest one corresponding to the DR.

In NPMM, only the fundamental fission neutron sources at the beginning of every cycle are utilized, and the higher mode information is from the statistical noises contained in the normalized neutron sources. Due to the strong inter-cycle correlation of the high DR problems, the NPMM requires many (usually thousands of) active cycles to get an accurate DR estimation or the first mode eigenvalue. For even higher eigenmodes, it requires even more active cycles for the NPMM to get the accurate eigenvalues, let alone the eigenvectors.

An obvious idea to get the higher mode results is to model them explicitly during the Monte Carlo simulation. It is expected that the number of active cycles required to get the accurate higher mode results can be greatly reduced. Besides, by extracting the higher modes from the fundamental mode, the convergence of the fundamental mode can be accelerated.

II. DESCRIPTION OF THE METHOD

The basics theory of the NPMM will be reviewed, followed by the extension method.

1. The Noise Propagation Matrix Method

During the Monte Carlo simulation, the fission source is a stochastic realization and can be described as:

$$\mathbf{s}^{(m)} = N\mathbf{s}_0 + \sqrt{N}\mathbf{e}^{(m)}, \tag{1}$$

where $\mathbf{s}^{(m)}$ is the fission source of cycle m, N is the number of histories per cycle, $\mathbf{s}_0$ is the expected normalized fundamental fission source, and $\mathbf{e}^{(m)}$ is the normalized stochastic noise representing the deviation of the cycle-m fission source from its expected value. Let $E[.]$ denote the expectation, there is:

$$E\left[\mathbf{s}^{(m)}\right] = N\mathbf{s}_0 \equiv \mathbf{s}. \tag{2}$$

For the noise term, there is:

$$E\left[\mathbf{e}^{(m)}\right] = 0. \tag{3}$$

The noise term of the source distribution is governed by a linear Markov process [1-8]:

$$\mathbf{e}^{(m)} = \mathbf{A}_0\mathbf{e}^{(m-1)} + \boldsymbol{\varepsilon}^{(m)}, \tag{4}$$

where $\mathbf{A}_0$ is called the NPM and $\boldsymbol{\varepsilon}^{(m)}$ represents the noise introduced to the neutron source during the neutron transport process at cycle-m. The following relationships hold:

$$\begin{aligned} &E\left[\boldsymbol{\varepsilon}^{(m)}\right] = 0, \\ &E\left[\boldsymbol{\varepsilon}^{(m1)}\mathbf{e}^{(m2)}\right] = 0,\ m1 > m2, \\ &E\left[\boldsymbol{\varepsilon}^{(m1)}\boldsymbol{\varepsilon}^{(m2)}\right] = 0,\ m1 \neq m2. \end{aligned} \tag{5}$$

Although the NPM is defined based on the noises, the practical implementations of the NPMM and CMPM use an alternative way utilizing the correlation matrices based on the fission sources. According to Eqs. (1) and (4), and using the property [1-8]

$$\mathbf{A}_0\mathbf{s}_0 = 0, \tag{6}$$

it can be shown that the equation governing the propagation of fission source from cycle to cycle is:

$$\mathbf{s}^{(m)} = \mathbf{A}_0\mathbf{s}^{(m-1)} + \boldsymbol{\eta}^{(m)}, \tag{7}$$

where

$$\boldsymbol{\eta}^{(m)} = N\mathbf{s}_0 + \sqrt{N}\boldsymbol{\varepsilon}^{(m)}. \tag{8}$$

Multiplying Eq. (7) with $\mathbf{s}^{(m-1)T}$ from right and taking expectation results in:

$$E\left[\mathbf{s}^{(m)}\mathbf{s}^{(m-1)T}\right] = \mathbf{A}_0 E\left[\mathbf{s}^{(m-1)}\mathbf{s}^{(m-1)T}\right] + E\left[\boldsymbol{\eta}^{(m)}\mathbf{s}^{(m-1)T}\right]. \tag{9}$$

According to Eqs. (1), (3), (5) and (8), there is:

$$\begin{aligned} &E\left[\boldsymbol{\eta}^{(m)}\mathbf{s}^{(m-1)T}\right] \\ &= E\left[\left(N\mathbf{s}_0 + \sqrt{N}\boldsymbol{\varepsilon}^{(m)}\right)\left(N\mathbf{s}_0 + \sqrt{N}\mathbf{e}^{(m-1)}\right)^T\right] \\ &= \mathbf{s}\mathbf{s}^T. \end{aligned} \tag{10}$$

Define the source correlation matrices as:

$$\mathbf{L}_0 \equiv E\left[\mathbf{s}^{(m)}\mathbf{s}^{(m)T}\right],\ \mathbf{L}_1 \equiv E\left[\mathbf{s}^{(m)}\mathbf{s}^{(m-1)T}\right]. \tag{11}$$

From Eqs. (9), (10) and (11), the NPM can be calculated:

$$\mathbf{A}_0 = \left[\mathbf{L}_1 - \mathbf{s}\mathbf{s}^T\right]\mathbf{L}_0^{-1}. \tag{12}$$

The largest-modulus eigenvalue of the NPM is the DR of the system.

2. Extension of the NPMM

The NPMM can be extended by looking at the fission source before and after the neutron transport process at one cycle.

The stationary fundamental fission source at the beginning of cycle-*m* can be written as:

$$\mathbf{v}_0^{(m)} = N\mathbf{v}_0 + \sqrt{N}\mathbf{e}_{00}^{(m)}, \tag{13}$$

while the corresponding fundamental mode fission produced neutron distribution at the end of cycle-*m* can be described as:

$$\mathbf{w}_0^{(m)} = k_0 N\mathbf{v}_0 + k_0\sqrt{N}\mathbf{e}_{01}^{(m)}, \tag{14}$$

where $\mathbf{v}_0$ is the expected normalized fundamental fission source, N is the number of neutron histories per cycle, k_0 is the fundamental mode eigenvalue, $\mathbf{e}_{00}^{(m)}$ and $\mathbf{e}_{01}^{(m)}$ are the normalized stochastic noise vectors that represent the deviation of the fundamental mode fission neutron distributions to their expected values at the beginning and end of cycle-*m*, respectively.

Since the power method is essentially adopted to solve the criticality eigenvalue problems with Monte Carlo, the fission neutron distributions relate to the power matrix, denoted as **P** in the equation:

$$\mathbf{w}_0 = \mathbf{P}\mathbf{v}_0 = k_0\mathbf{v}_0. \tag{15}$$

Similar to Eq. (4), the noise propagation equation can be written as:

$$k_0\mathbf{e}_{01}^{(m)} = \mathbf{P}\mathbf{e}_{00}^{(m)} + k_0\boldsymbol{\varepsilon}_0^{(m)}, \tag{16}$$

where $\boldsymbol{\varepsilon}_0^{(m)}$ is the stochastic noise introduced to the fundamental mode neutron distribution at cycle-*m*. According to Eqs. (14), (15) and (16), it can be derived that:

$$\mathbf{w}_0^{(m)} = \mathbf{P}\mathbf{v}_0^{(m)} + k_0\sqrt{N}\boldsymbol{\varepsilon}_0^{(m)}. \tag{17}$$

Similarly, if the *i*-th mode neutron source can be simulated explicitly, the *i*-th mode fission neutron distributions at the beginning and end of cycle-*m* can be related with the following equation:

$$\mathbf{w}_i^{(m)} = \mathbf{P}\mathbf{v}_i^{(m)} + k_i\sqrt{N}\boldsymbol{\varepsilon}_i^{(m)}, \tag{18}$$

where k_i is the *i*-th mode eigenvalue and $\boldsymbol{\varepsilon}_i^{(m)}$ is the stochastic noise introduced to *i*-th mode neutron source during cycle-*m*.

According to Eqs. (17) and (18), if the first N eigenmode fission sources are simulated explicitly, there is:

$$\left(\mathbf{w}_0^{(m)},\cdots,\mathbf{w}_{N-1}^{(m)}\right)=\mathbf{P}\left(\mathbf{v}_0^{(m)},\cdots,\mathbf{v}_{N-1}^{(m)}\right) + \sqrt{N}\left(k_0\boldsymbol{\varepsilon}_0^{(m)},\cdots,k_{N-1}\boldsymbol{\varepsilon}_{N-1}^{(m)}\right), \tag{19}$$

which can be further written in the matrix form as:

$$\mathbf{W}^{(m)}=\mathbf{P}\mathbf{V}^{(m)}+\mathbf{U}^{(m)}. \tag{20}$$

Since the stochastic noises introduced during cycle-m are independent of the neutron sources at the beginning of cycle, similar to Eq. (5), there is:

$$E\left[\mathbf{U}^{(m)}\mathbf{V}^{(m)T}\right]=0. \tag{21}$$

Multiplying Eq. (20) with $\mathbf{V}^{(m)T}$ from right and taking the expectation results in:

$$E\left[\mathbf{W}^{(m)}\mathbf{V}^{(m)T}\right]=\mathbf{P}\cdot E\left[\mathbf{V}^{(m)}\mathbf{V}^{(m)T}\right]. \tag{22}$$

The power matrix can then be calculated as:

$$\mathbf{P}=E\left[\mathbf{W}^{(m)}\mathbf{V}^{(m)T}\right]\left\{E\left[\mathbf{V}^{(m)}\mathbf{V}^{(m)T}\right]\right\}^{-1}. \tag{23}$$

It can be noticed that the eigenvalues of the power matrix are the eigenvalues of the system, while its eigenvectors are the different mode fission sources.

3. Implementation of the extended NPMM

The main improvement of the ENPMM is to simulate the higher mode fission sources explicitly. This was done by introduce multiple weights to one neutron. Neutrons with both positive and negative weights should be modeled for higher mode fission sources, so a weight cancellation procedure is required. In this study, the fine mesh average based weight cancellation was adopted, the same as the authors adopted in previous works about the MPM [9-11].

During the simulation, the source correlation matrices are accumulated:

$$\mathbf{L}_0^{(m)}=\sum_{i=m_0+1}^{m}\mathbf{V}^{(i)}\mathbf{V}^{(i)T},\ \mathbf{L}_1^{(m)}=\sum_{i=m_0+1}^{m}\mathbf{W}^{(i)}\mathbf{V}^{(i)T}, \tag{24}$$

where m_0 is the number of cycles skipped before accumulation of the correlation matrices. The cycle-*m* estimated power matrix is then calculated as:

$$\mathbf{P}^{(m)}=\mathbf{L}_1^{(m)}\left(\mathbf{L}_0^{(m)}\right)^{-1}. \tag{25}$$

The power matrix is then eigen-decomposed:

$$\mathbf{P}^{(m)}=\mathbf{Q}^{(m)}\mathbf{\Lambda}^{(m)}\left(\mathbf{Q}^{(m)}\right)^{-1}, \tag{26}$$

where the columns of $\mathbf{Q}^{(m)}$ are the eigenvectors of $\mathbf{P}^{(m)}$, and $\mathbf{\Lambda}^{(m)}$ is a diagonal matrix which contains the eigenvalues of $\mathbf{P}^{(m)}$. The first *N* eigenvectors are used to calculate the updating factors for the fission sources:

$$\mathbf{W}^{(m)}\mathbf{X}^{(m)}=\mathbf{Q}^{(m)}\left(:,1:N\right), \tag{27}$$

where $\mathbf{W}^{(m)}$ is a *M*-by-*N* matrix, *M* is the number of meshes used to discretize the space, *M*>*N*, $\mathbf{X}^{(m)}$ is a *N*-by-*N* matrix, and it can be calculated with the least square method.

III. RESULTS

1. The 2D Square Problem

The multi-group 2D homogeneous square neutron transport problem was modeled first to demonstrate the ENPMM. 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 2D square is 400 cm, with black boundary on four sides. The 5x5 uniform coarse meshes were used to discretize the fission sources, and 8 or 16 eigenmodes were simulated at the same time. The Monte Carlo simulations were done with 400 inactive cycles, 400 active cycles and 500,000 histories per cycle. The results are shown in Figs. 1-5.

The fission sources were initialized randomly in the whole space. Fig. 1 shows that finally all the simulations converged to the same fundamental mode fission source, and the ENPMM results show some source convergence acceleration effect. The eigenvalues shown in Figs. 2 and 3 present very big fluctuation at the beginning cycles. As more cycles simulated, more source correlation matrices are accumulated, so the affection of the stochastic noises is reduced and the eigenvalues become stable. The eigenvalue spectrum shown in Fig. 4 confirms the correctness of the first 16 eigenmode solutions. The fission source eigenmodes shown in Fig. 5 are also reasonable.

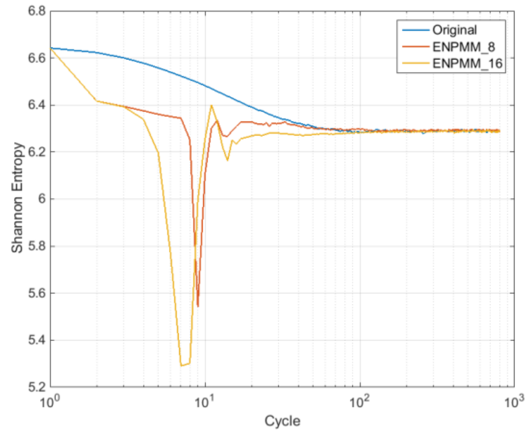

Fig. 1. The Shannon Entropy results.

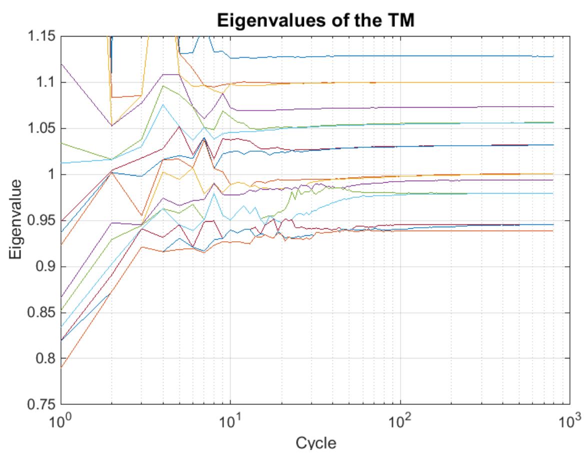

Fig. 2. Eigenvalues of the power matrix (TM, transfer matrix).

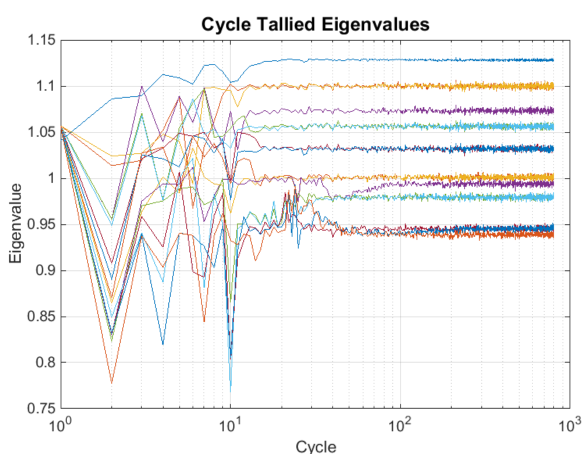

Fig. 3. Eigenvalues tallied at every cycle. They are calculated as the ratio of the total absolute weight to the total starting number of histories.

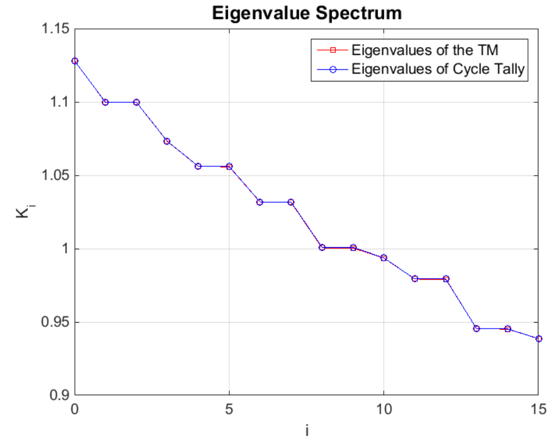

Fig. 4. The eigenvalue spectrum.

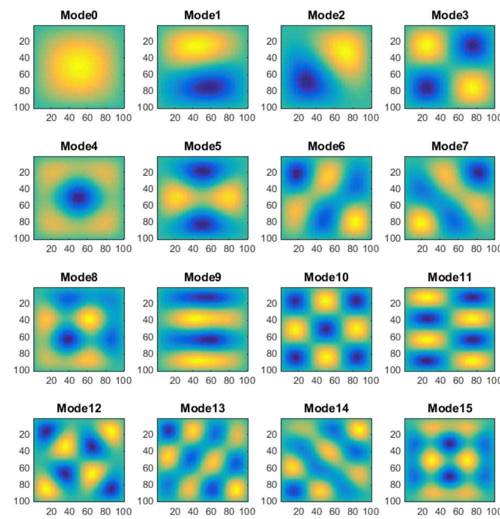

Fig. 5. The first 16 fission source eigenmodes.

2. The 3D Cube Problem

The multi-group 3D homogeneous cube neutron transport problem was modeled to further demonstrate the performance of the ENPMM. This problem features degeneracy of multiplicity of 3 and 6. 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 were used to discretize the system space. The Monte Carlo simulations were done with 100 inactive cycles, 300 active cycles and 500,000 histories per cycle.

Fig. 6 shows that the eigenvalues of the power matrix fluctuate a lot at the beginning cycles, and become stable due to the accumulation as more cycles are simulated. Fig. 7 also shows the same phenomenon. The eigenvectors of the power matrix were used to correct the neutron weights since cycle 10. The tallied eigenvalues at the following cycles fluctuate a lot, but they become stable finally when more cycles are simulated. The eigenvalue spectrum shown in Fig. 8 confirms the correctness of the eigenvalue results.

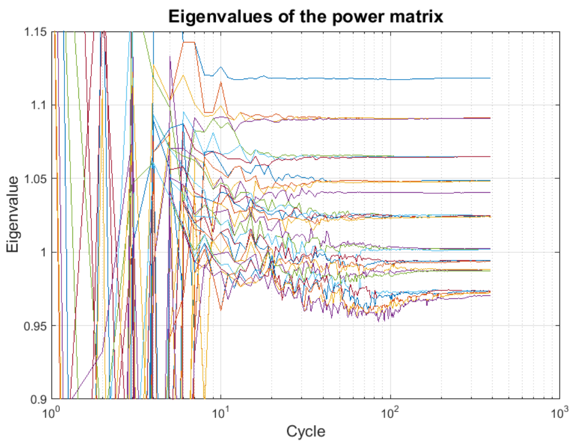

Fig. 6. The eigenvalues of the power matrix.

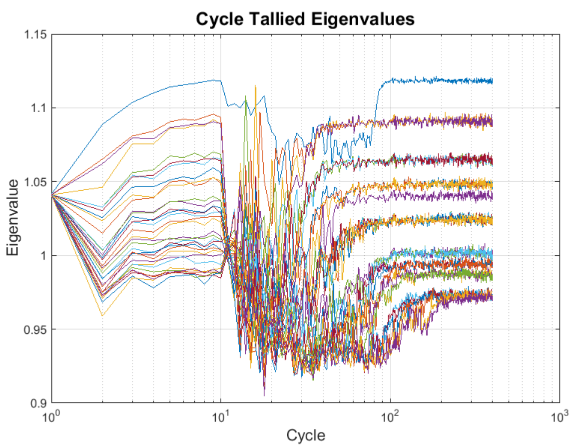

Fig. 7. The eigenvalues tallied at every cycle.

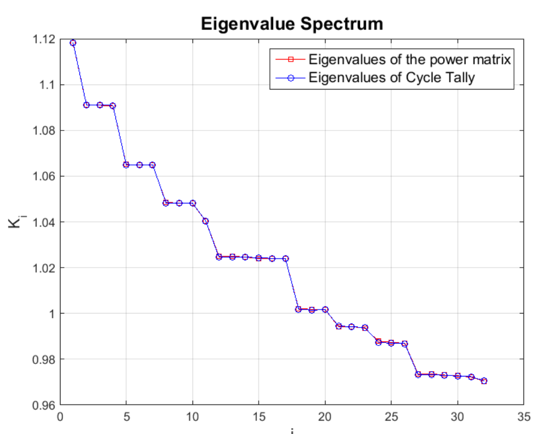

Fig. 8. The eigenvalue spectrum.

3. The 2D Checkboard Problem

The problem geometry is shown in Fig. 9. The same problem has also been modeled by Sutton [1] and Ueki et al [4-5]. The ENPMM results are shown in Figs. 10-14. The simulations were done with 300 inactive cycles, 600 active cycles and 200,000 histories per cycle. The 9x9 uniform coarse meshes were used for the space discretization.

Figs. 10 and 11 confirm that the ENPMM can give accurate higher mode eigenvalues by modeling the corresponding eigenmodes explicitly. In Fig. 10, only the first 4 eigenvalues are stable, while in Fig. 11 all the 10 eigenvalues are stable. The calculate DR is around 0.9982 using the first two eigenvalues (k_0=1.07090±0.00004, k_1=1.06899±0.00012), which is consistent with the results of Sutton and Ueki et al. Fig. 12 confirms that all the ENPMM simulations finally converge to the same fundamental fission source. The eigenvalue spectrum shown in Fig. 13 confirms the correctness of the eigenvalue results. Fig. 14 shows the first 10 fission source eigenmodes and they are reasonable.

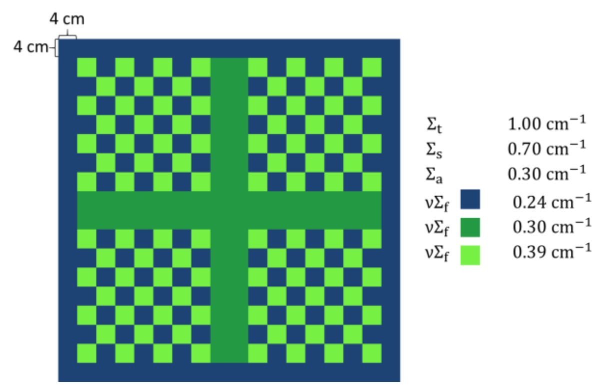

Fig. 9. The geometry and nuclear data of the 2D checkboard problem.

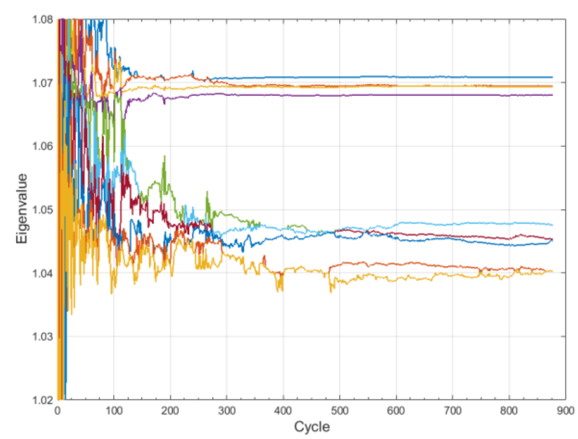

Fig. 10. The first 10 eigenvalues of the ENPMM with 4 modes.

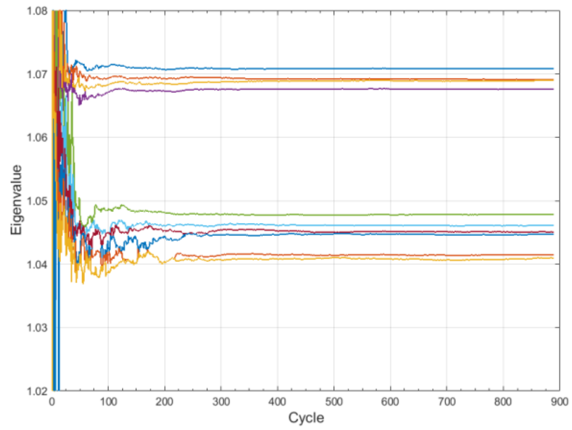

Fig. 11. The first 10 eigenvalues of the ENPMM with 10 modes.

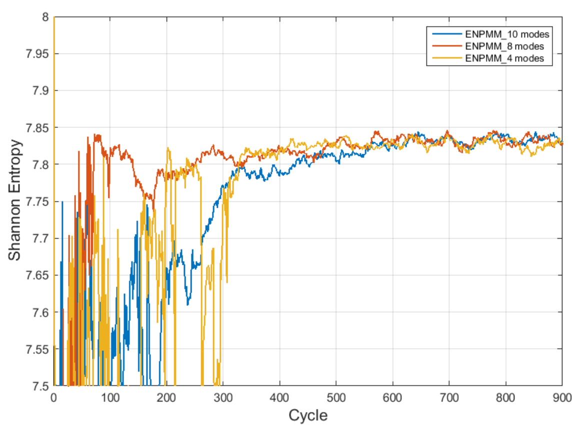

Fig. 12. The Shannon Entropy results of the ENPMM with different number of modes.

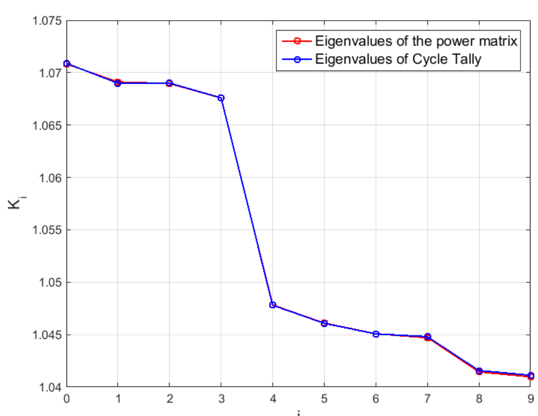

Fig. 13. The eigenvalue spectrum.

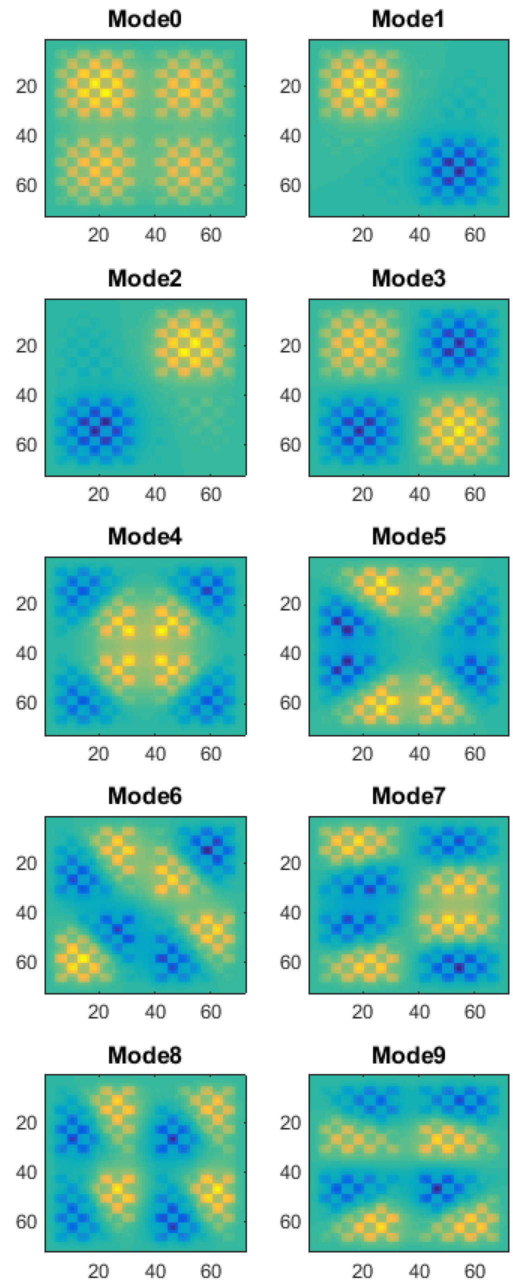

Fig. 14. The first 10 fission source eigenmodes of the ENPMM with 10 modes.

IV. CONCLUSIONS

The extended noise propagation matrix method (ENPMM) has been proposed. It is built upon the general description of the Monte Carlo implementation of the power method, that is, a power matrix is implicitly modeled while there is stochastic noise introduced during the power operation. As the stochastic noises introduced during one cycle is independent of the neutron sources to start the cycle, the accumulation of the source correlation matrices is used to alleviate the impact of the noises, and to get stable and accurate power matrix and the eigenmode solutions as more and more cycles are simulated.

The numerical tests successfully demonstrate the performance of the ENPMM. The results confirm that the higher mode solutions can be obtained accurately by modeling the corresponding eigenmodes explicitly. Further study should be conducted to investigate the performance of the ENPMM for practical 3D whole core problems.

ACKNOWLEDGMENTS

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