



## Original Article

# Calculation of Degenerated Eigenmodes with Modified Power Method

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## ABSTRACT

The modified power method has been studied by many researchers to calculate the higher eigenmodes and accelerate the convergence of the fundamental mode. Its application to multidimensional problems may be unstable due to degenerated or near-degenerated eigenmodes. Complex eigenmode solutions are occasionally encountered in such cases, and the shapes of the corresponding eigenvectors may change during the simulation. These issues must be addressed for the successful implementation of the modified power method. Complex components are examined and an approximation method to eliminate the usage of the complex numbers is provided. A technique to fix the eigenvector shapes is also provided. The performance of the methods for dealing with those aforementioned problems is demonstrated with two dimensional one group and three dimensional one group homogeneous diffusion problems.

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## 1. Introduction

The *power method* has been widely used to calculate the fundamental mode of the eigenvalue problem, with the convergence rate determined by the dominance ratio. The power iteration can be done as an outer iteration in deterministic calculations adopting inner and outer iterations, or as the simulation of one cycle of particles in Monte Carlo simulations.

The power method can calculate the higher modes only when the lower order forward and adjoint eigenvectors are

known. The modified power method (MPM) was recently developed to calculate the first several eigenmodes of the eigenvalue problem at the same time, and to accelerate the convergence of the fundamental mode.

The basic idea of the MPM is to force the local eigenvalues of different subregions to be the same. Booth [1], Gubernatis and Booth [2] and Booth and Gubernatis [3–6] were the first to propose this idea, and they developed the method for obtaining the first two eigenmodes at the same time. Booth [1] also proposed a similar method for the third and even higher eigenmodes, but this method required solving a

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higher order polynomial equation, which may be not practical for application. Zhang et al. [7–10] extended the originally proposed MPM, and provided a general solution strategy, in which a transfer matrix (TM) was introduced to help solve the first several eigenmodes. The eigenvalues of the TM are the eigenvalues of the system, while the eigenvectors of the TM are the eigenvectors of the system integrated over coarse meshes.

At the end of every iteration of the MPM, the eigen-decomposition of the TM should be done, and then the eigenvectors of the TM will be used to modify the neutron sources. In cases where there are multiple eigenmodes corresponding to the same eigenvalue or when two successive eigenvalues are so close that they cannot be distinguished, the eigen-decomposition may give complex conjugate eigensolutions, which cannot be used to update the neutron sources. A similar problem was also encountered in other studies that were based on eigen-decomposition of the matrix [11]. Another problem is that for the eigenmodes with the same eigenvalue, the eigen-decomposition may give different eigenvectors every time, which may cause a problem for the convergence of the eigenvectors.

Section 2 of this paper gives a general review on the theory of MPM. In Section 3, the degeneracy issues are accounted, while the numerical tests and discussions will be given in Section 4. Finally, the conclusions are given in Section 5.

## 2. Review of the MPM

The basic idea of the MPM is that the multiple local eigenvalues should be the same if the eigenfunction converges, and the convergence of the eigenfunction can be accelerated by forcing the multiple local eigenvalues to be the same.

If the first two eigenmodes are to be solved, the simulation should start with two initial functions:

$$\psi_1 = \sum_i a_i \phi_i, \quad \psi_2 = \sum_i b_i \phi_i, \quad i = 0, 1, 2, \dots, \quad (1)$$

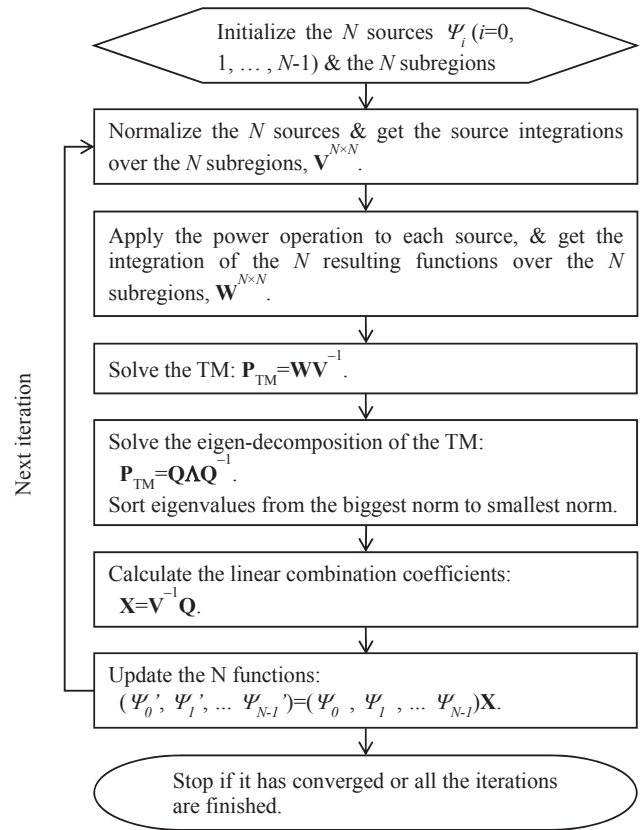
where  $\phi_i$  is the eigenfunction, and  $a_i$  and  $b_i$  are the expansion coefficients of the two initial functions. Applying power operation  $A$  to the two initial functions will give:

$$A\psi_1 = \sum_i a_i k_i \phi_i, \quad A\psi_2 = \sum_i b_i k_i \phi_i, \quad i = 0, 1, 2, \dots, \quad (2)$$

where  $k_i$  is the eigenvalue. The local eigenvalues can be defined as:

$$k^{i,j} = \frac{\int_{R_j} A\psi_i dr}{\int_{R_j} \psi_i dr} = \frac{W_{ji}}{V_{ji}}, \quad (3)$$

where  $k^{i,j}$  is the eigenvalue defined over subregion  $R_j$  and calculated with the  $i$ th function, and  $V_{ji}$  and  $W_{ji}$  are the integrations of the  $i$ th function over subregion  $R_j$  before and



**Fig. 1 – The flow chart of the general solution strategy of modified power method.**

after the power operation. The local eigenvalues are forced to be the same by the linear combination of the two functions:

$$k = k^j = \frac{\int_{R_j} (xA\psi_1 + yA\psi_2) dr}{\int_{R_j} (x\psi_1 + y\psi_2) dr} = \frac{xW_{j1} + yW_{j2}}{xV_{j1} + yV_{j2}}, \quad j = 1, 2, \dots, \quad (4)$$

Two sets of solution  $(k, x, y)$  will be obtained and they will satisfy:

$$\begin{pmatrix} W_{11} & W_{12} \\ W_{21} & W_{22} \\ \vdots & \vdots \end{pmatrix} \begin{pmatrix} x_1 & x_2 \\ y_1 & y_2 \end{pmatrix} = \begin{pmatrix} V_{11} & V_{12} \\ V_{21} & V_{22} \\ \vdots & \vdots \end{pmatrix} \begin{pmatrix} x_1 & x_2 \\ y_1 & y_2 \end{pmatrix} \begin{pmatrix} k_0 & 0 \\ 0 & k_1 \end{pmatrix}, \quad (5)$$

$$\mathbf{WX} = \mathbf{VXA},$$

where  $\mathbf{V}$  and  $\mathbf{W}$  are the function integrals before and after the power operation,  $\mathbf{X}$  is the coefficient matrix, and  $\mathbf{\Lambda}$  is the diagonal matrix containing the eigenvalues. To solve the

**Table 1 – The one-group cross sections.**

$\Sigma_a$ (cm <sup>-1</sup> )	$\nu\Sigma_f$ (cm <sup>-1</sup> )	D (cm)
0.2	0.3	1/3

two solution sets, two independent subregions are needed in this case.

The method described above can be extended to get the first  $N$  eigenmodes at the same time. To solve the  $N$  solution sets,  $N$  independent subregions should be predefined. The following linear system should be solved:

$$\begin{pmatrix} W_{11} & \dots & W_{1N} \\ \vdots & \ddots & \vdots \\ W_{N1} & \dots & W_{NN} \end{pmatrix} \begin{pmatrix} x_{11} & \dots & x_{1N} \\ \vdots & \ddots & \vdots \\ x_{N1} & \dots & x_{NN} \end{pmatrix} = \begin{pmatrix} V_{11} & \dots & V_{1N} \\ \vdots & \ddots & \vdots \\ V_{N1} & \dots & V_{NN} \end{pmatrix} \begin{pmatrix} x_{11} & \dots & x_{1N} \\ \vdots & \ddots & \vdots \\ x_{N1} & \dots & x_{NN} \end{pmatrix} \begin{pmatrix} k_0 & \dots & 0 \\ \vdots & \ddots & \vdots \\ 0 & \dots & k_{N-1} \end{pmatrix}, \quad (6)$$

$$WX = VX\Lambda.$$

To solve Eq. (6), it can be transformed into:

$$W = VX\Lambda X^{-1} = VX\Lambda(VX)^{-1}V = P_{TM}V, \quad (7)$$

where  $P_{TM}[\triangleq VX\Lambda(VX)^{-1}]$  is called the TM in this study. It can be seen that the TM can be calculated with the function

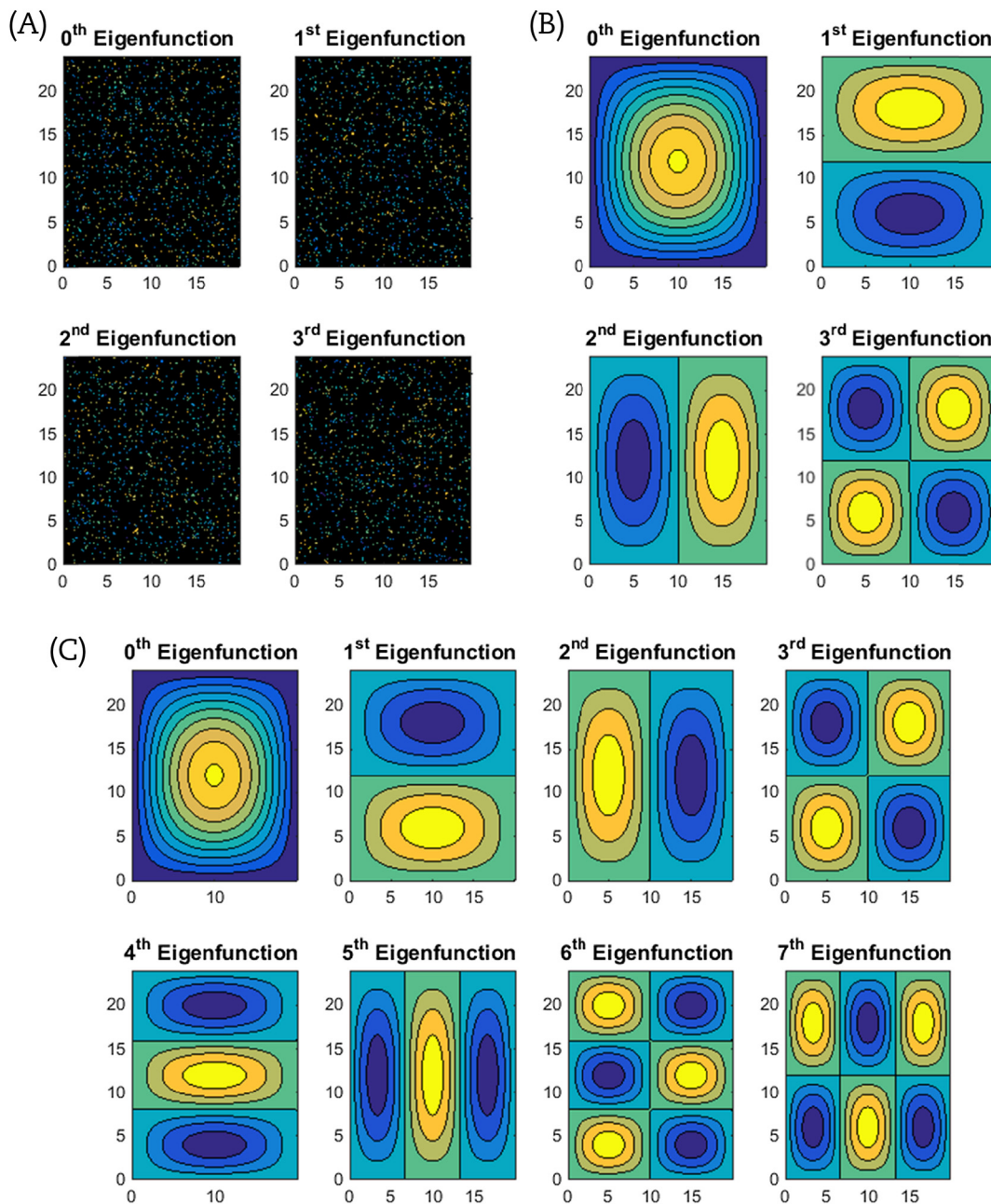


Fig. 2 – The 2D rectangle problem. (A) The initial random functions; (B) final functions; and (C) reference eigenfunctions.

integrals before and after the power operation, and its eigenvalues are the eigenvalues of the system, while its eigenvectors are the eigenfunction integrals over the subregions. The TM is often confused with a fission matrix [12,13] although they have fundamentally different characteristics especially for higher harmonics, and therefore a thorough investigation of the characteristics of the TM has been performed which will be published in a separate journal article [14] (currently under review). The solution strategy of the MPM can be described with the flow chart shown in Fig. 1.

### 3. Accounting for the degeneracy issues

According to the description of the previous section, the TM should be solved and the eigen-decomposition of the TM should be done at the end of every iteration. For problems in which all the eigenvalues are different, the MPM works very well. However, it may be unstable if the problem has degenerated intermediate eigenmode solutions.

#### 3.1. The complex intermediate eigenmode solutions

In some cases, the complex eigenmode solutions of the TM are frequently encountered during the simulation, and the eigenvectors cannot be used to update the eigenfunctions. Just

skipping the current iteration without updating the eigenfunctions does not work, as the complex solutions are encountered again later. An approximation to real eigenpairs (ARE) has been developed to solve this problem.

If the TM has a complex eigenvalue  $(\lambda_R + i\lambda_I)$  with eigenvector  $(\mathbf{u}_R + i\mathbf{u}_I)$ , they, together, should satisfy:

$$\mathbf{P}_{TM}(\mathbf{u}_R + i\mathbf{u}_I) = (\lambda_R + i\lambda_I)(\mathbf{u}_R + i\mathbf{u}_I), \quad (8)$$

where  $\mathbf{u}_R$  and  $\mathbf{u}_I$  are real vectors,  $\lambda_R$  and  $\lambda_I$  are real numbers and  $i$  is the imaginary unit. Taking the complex conjugate of both sides, and noting that the TM is a real matrix, it gives:

$$\mathbf{P}_{TM}(\mathbf{u}_R - i\mathbf{u}_I) = (\lambda_R - i\lambda_I)(\mathbf{u}_R - i\mathbf{u}_I). \quad (9)$$

Therefore, the complex eigenvalues and eigenvectors should be in the form of complex conjugate pairs. The real and imaginary parts of the eigenvectors,  $\mathbf{u}_R$  and  $\mathbf{u}_I$ , should be independent. Otherwise, there is  $\mathbf{u}_I = C\mathbf{u}_R$ , and according to Eqs. (8) and (9):

$$\begin{aligned} \mathbf{P}_{TM}\mathbf{u}_R &= (\lambda_R + i\lambda_I)\mathbf{u}_R, \\ \mathbf{P}_{TM}\mathbf{u}_R &= (\lambda_R - i\lambda_I)\mathbf{u}_R. \end{aligned} \quad (10)$$

Therefore,  $\lambda_I = 0$ . Actually  $\lambda_I \neq 0$ , so  $\mathbf{u}_R$  and  $\mathbf{u}_I$  are independent.

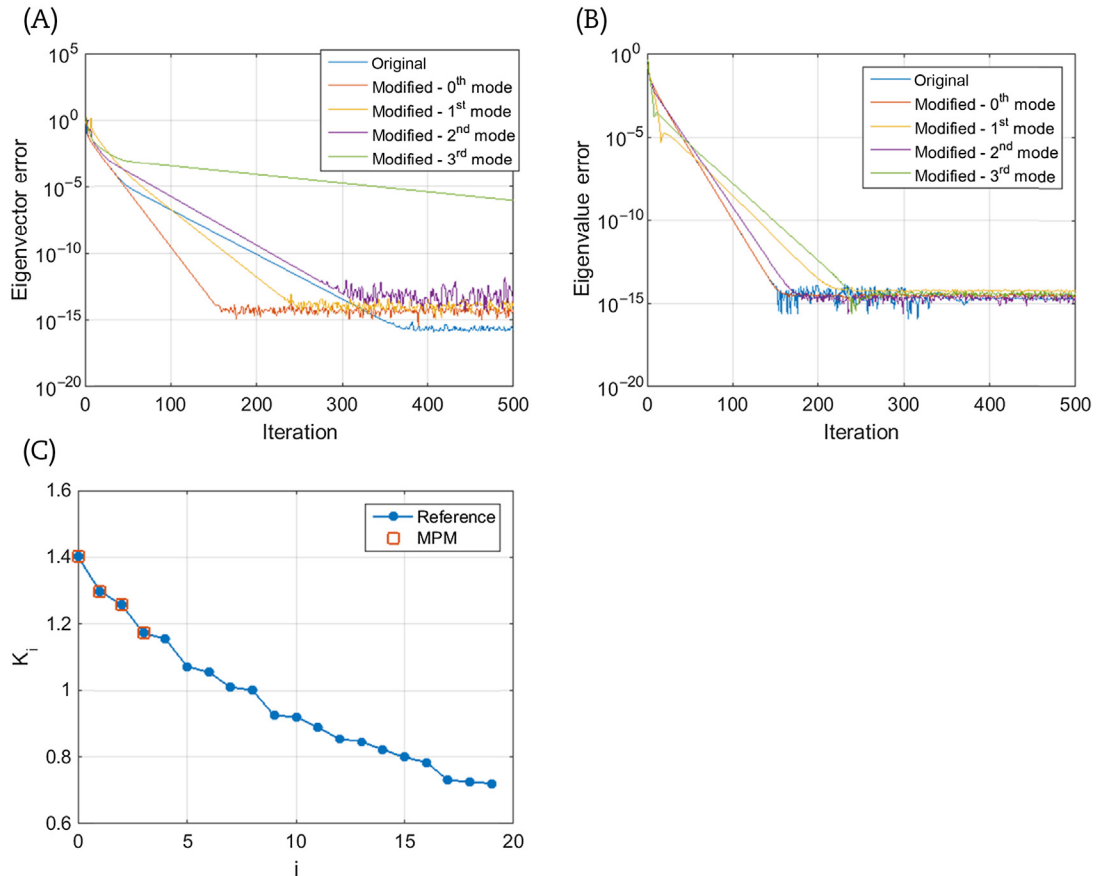
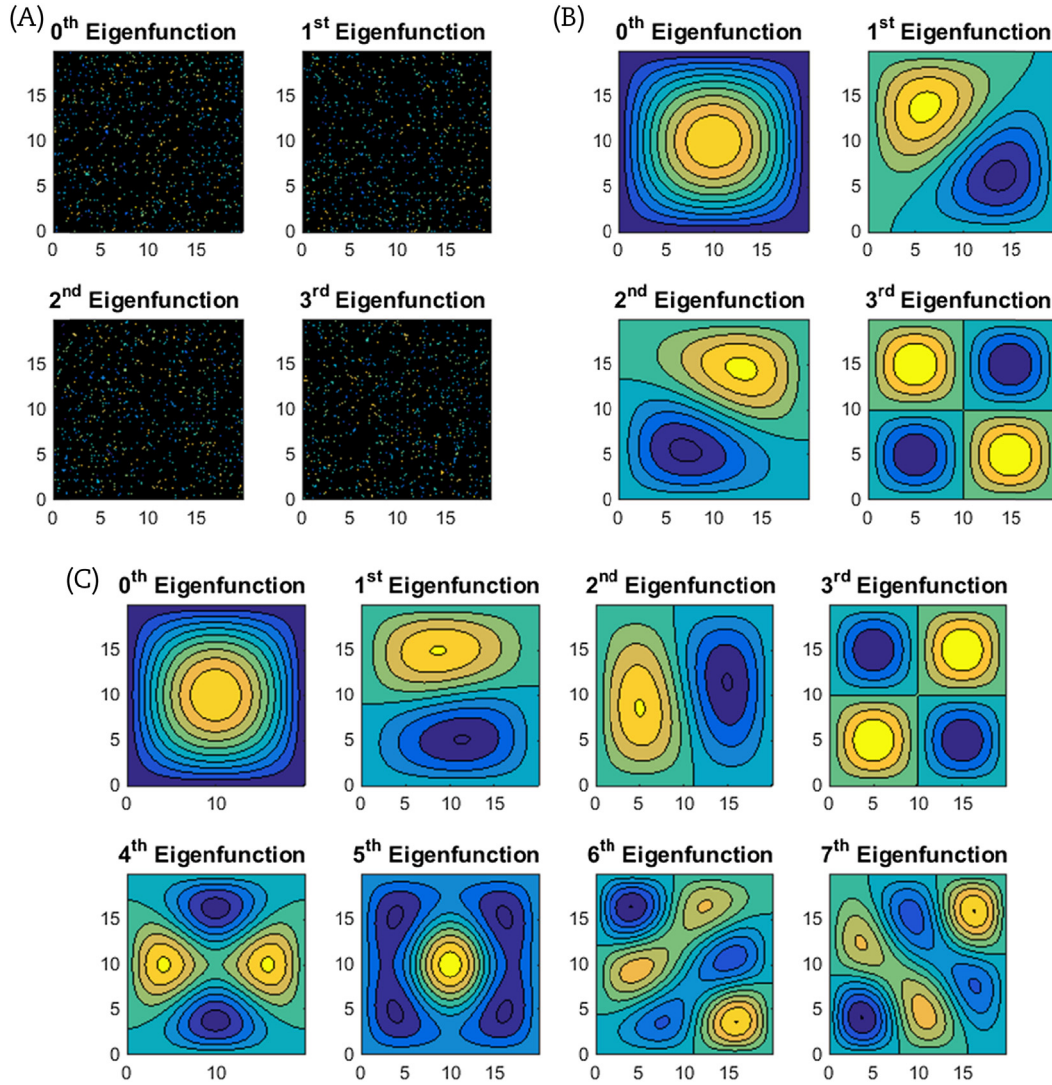


Fig. 3 – The modified power method (MPM) results of the 2D rectangle problem. (A) The eigenvector errors; (B) eigenvalue errors; and (C) eigenvalue spectrum.



**Fig. 4 – The 2D square problem. (A) The initial random functions; (B) final functions; and (C) reference eigenfunctions.**

In addition, it is noted that usually  $|\lambda_i| \ll |\lambda_R|$  and  $\lambda_i$  are decreasing during the simulation. Considering that the degenerated eigenmodes of the power operation matrix  $\mathbf{A}$  have the same eigenvalue, it is natural that  $\lambda_R$  should be a good approximation of the eigenvalue. Taking the addition and subtraction of the Eqs. (8) and (9) yields:

$$\begin{aligned} \mathbf{P}_{TM} \mathbf{u}_R &= \lambda_R \mathbf{u}_R - \lambda_I \mathbf{u}_I \approx \lambda_R \mathbf{u}_R, \\ \mathbf{P}_{TM} \mathbf{u}_I &= \lambda_R \mathbf{u}_I + \lambda_I \mathbf{u}_R \approx \lambda_R \mathbf{u}_I. \end{aligned} \quad (11)$$

It can be seen from Eq. (11) that the linearly independent vectors  $\mathbf{u}_R$  and  $\mathbf{u}_I$  can be taken as the two approximated eigenvectors.

### 3.2. The shape fixing of the degenerated eigenvectors

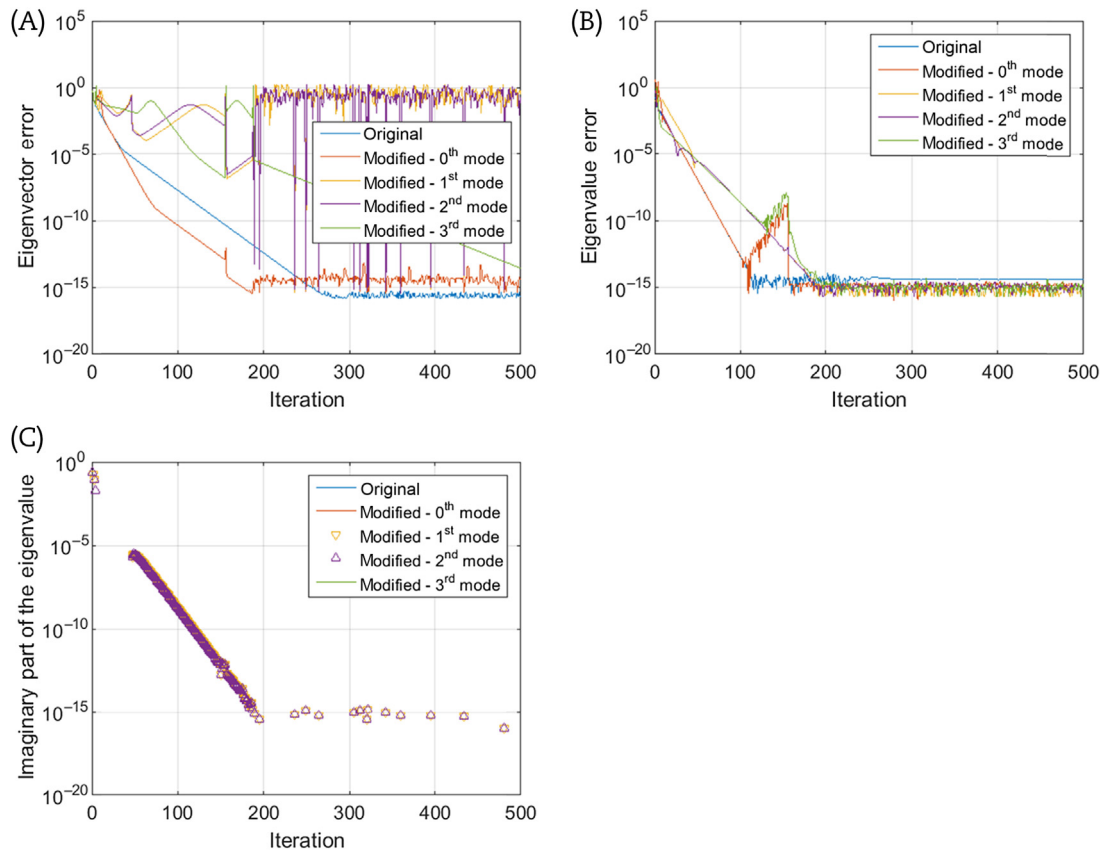
Another problem for the degenerated eigenmodes is that the eigen-decomposition of the TM gives different corresponding eigenvectors every time, and so the corresponding columns of the  $\mathbf{X}$  matrix are also different. Updating the distributions

with this  $\mathbf{X}$  matrix will introduce large errors in the eigenvectors if no constraints are provided.

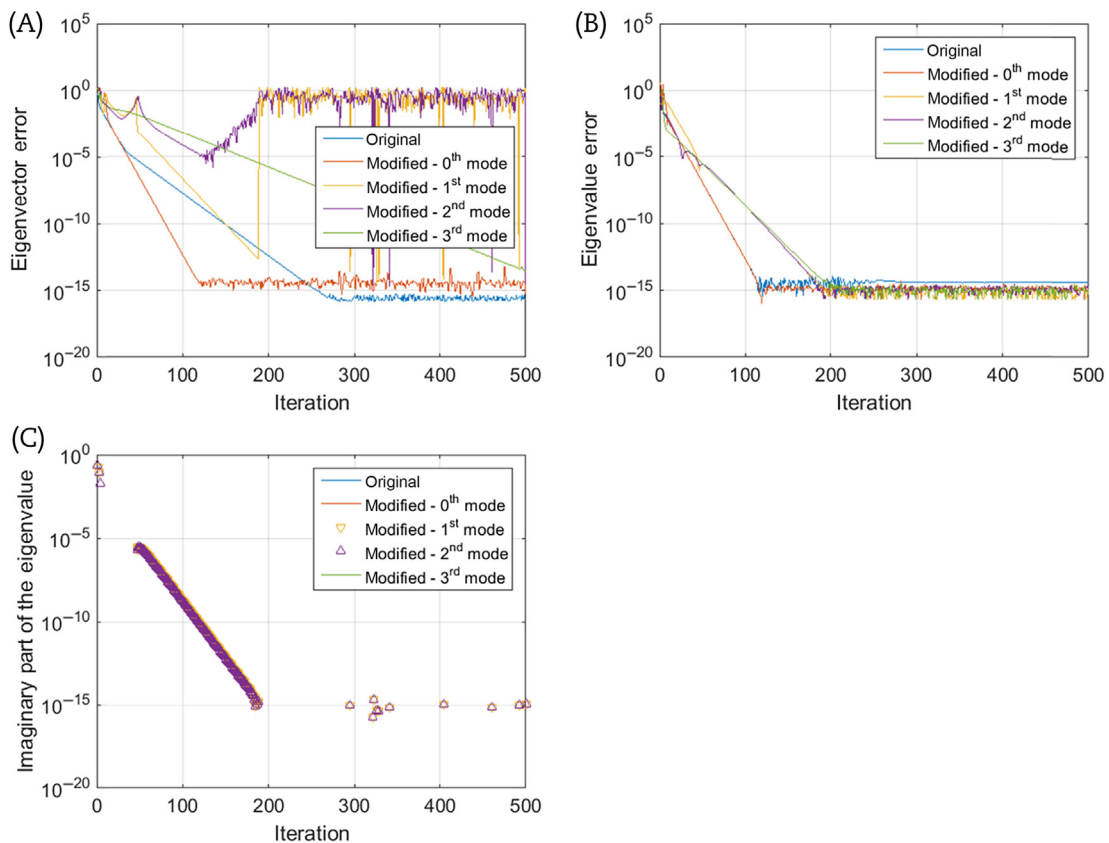
In cases where all the eigenvectors are fixed, the  $\mathbf{X}$  matrix will finally converge on the identity matrix, which means no compensation from other modes is necessary. Therefore, a logical idea to fix the shapes of the degenerated eigenvectors is to avoid the mixing of the corresponding sources.

The element of the  $\mathbf{X}$  matrix,  $x_{ji}$ , represents the compensation from the  $j$ -th source distribution to the  $i$ -th source distribution. If the  $i$ -th and  $j$ -th eigenmodes are degenerated, the mixing of the  $i$ -th and  $j$ -th source distributions should be avoided, which means  $x_{ji}$  and  $x_{ij}$  should be 0. They cannot be set as 0 directly, but they can become 0 by combining the two columns of the  $\mathbf{X}$  matrix:

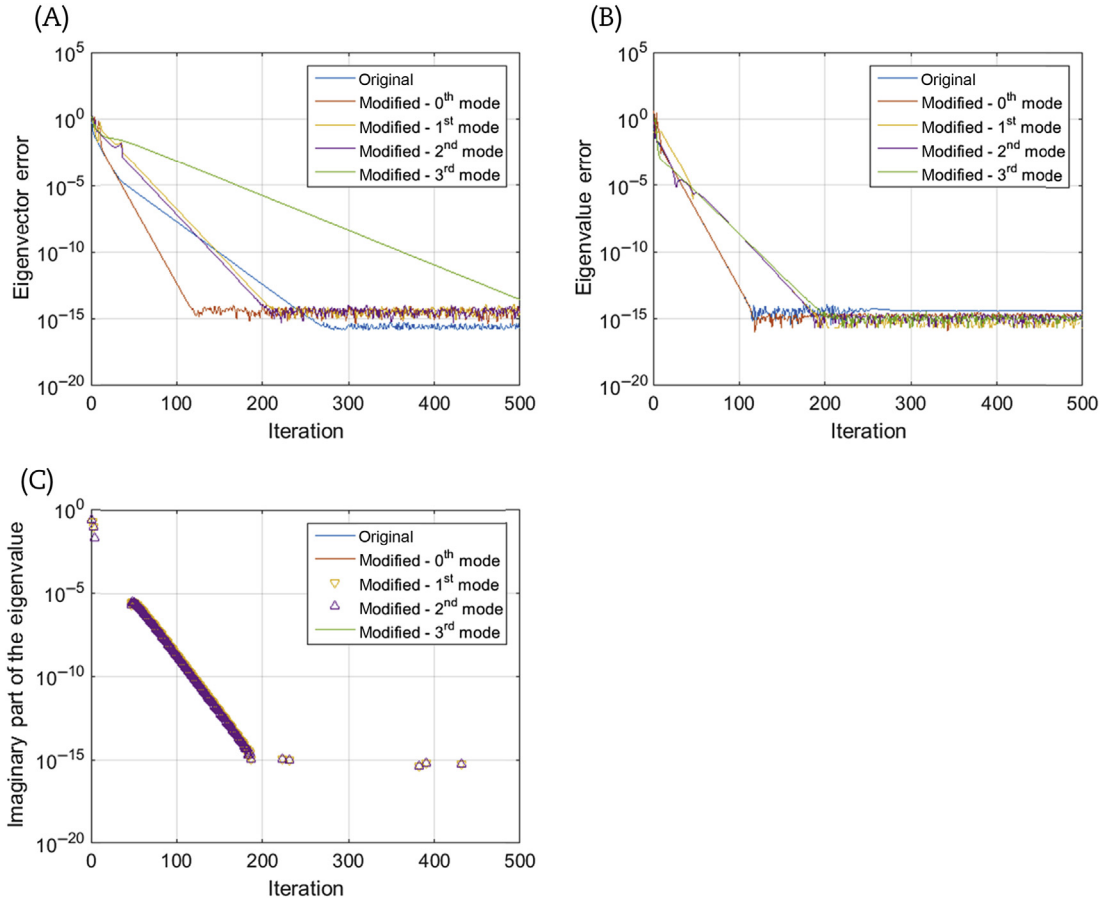
$$\begin{pmatrix} \vdots & \vdots \\ x_{ii} & x_{ij} \\ \vdots & \vdots \\ x_{ji} & x_{jj} \\ \vdots & \vdots \end{pmatrix} \begin{pmatrix} f_{ii} & f_{ij} \\ f_{ji} & f_{jj} \end{pmatrix} = \begin{pmatrix} \vdots & \vdots \\ 1 & 0 \\ \vdots & \vdots \\ 0 & 1 \\ \vdots & \vdots \end{pmatrix}, \quad (12)$$



**Fig. 5 – The results of the 2D square without approximation to real eigenpairs. (A) The eigenvector errors; (B) eigenvalue errors; and (C) imaginary parts of the eigenvalues of the TM. TM, transfer matrix.**



**Fig. 6 – The results of the 2D square without basis vector fixing. (A) The eigenvector errors; (B) eigenvalue errors; and (C) imaginary parts of the eigenvalues of the TM. TM, transfer matrix.**



**Fig. 7 – The results of the 2D square with both approximation to real eigenpairs and basis vector fixing. (A) The eigenvector errors; (B) eigenvalue errors; and (C) the imaginary parts of eigenvalues of the TM. TM, transfer matrix.**

where  $f$  is the linear combination factors, and

$$\begin{pmatrix} f_{ii} & f_{ij} \\ f_{ji} & f_{jj} \end{pmatrix} = \begin{pmatrix} x_{ii} & x_{ij} \\ x_{ji} & x_{jj} \end{pmatrix}^{-1}.$$

In practice there may be degeneracy with multiplicity of more than 2. After the eigen-decomposition of the TM, the eigenvalues are put in order from the largest norm to the smallest norm, and the corresponding eigenvectors are also re-ordered. The degenerated eigenmodes are checked based on the differences of the eigenvalues. If the  $i_b$ -th to  $i_e$ -th eigenmodes are degenerated, the coefficient matrix  $\mathbf{X}$  is modified with:

$$\mathbf{X}(:, i_b : i_e) = \mathbf{X}(:, i_b : i_e) \cdot \mathbf{X}(i_b : i_e, i_b : i_e)^{-1}. \quad (13)$$

After this modification, there will be no mixing among the  $i_b$ -th to  $i_e$ -th source distributions when  $\mathbf{X}$  is applied to update the neutron sources. This will be referred to as the technique of basis vector fixing (BVF) in degenerated eigen-space in the following discussion.

#### 4. The numerical tests and discussion

In order to test and show the effects of the techniques described above, the monoenergetic homogeneous diffusion problems are modeled. The diffusion equation to be solved is:

$$-D\nabla^2\phi(r) + \Sigma_a\phi(r) = \frac{1}{k}\nu\Sigma_f\phi(r), \quad (14)$$

where  $D$  is the diffusion coefficient,  $\Sigma_a$  is the absorption cross section, and  $\nu\Sigma_f$  is the product of the number of neutrons produced per fission and the fission cross section.

The 1G cross sections are listed in Table 1. The black boundary conditions are adopted for all boundaries. Finite difference method is adopted to solve Eq. (14) numerically, which can be discretized into the matrix form:

$$\mathbf{M}\phi = \frac{1}{k}\mathbf{F}\phi, \quad (15)$$

where  $\mathbf{M}$  is a tri-, five-, or seven-diagonal matrix for one dimensional, two dimensional or three dimensional systems representing the leakage and absorption terms, while  $\mathbf{F}$  is a diagonal matrix representing the fission production term. The power operator matrix  $\mathbf{A}$  is constructed with fine meshes as:

$$\begin{aligned} \mathbf{A} &= \mathbf{M}^{-1}\mathbf{F}, \\ \mathbf{A}\phi &= k\phi. \end{aligned} \quad (16)$$

Consequently, the reference solutions can be obtained with the direct eigen-decomposition of the matrix  $\mathbf{A}$ . The power iteration consists of multiplying  $\mathbf{A}$  and the flux vector  $\phi$  once, and then updating the eigenvalue  $k$ . For all cases, the iteration will be done 500 times, whether the solutions are converged or not.

4.1. 20 cm × 24 cm 2D rectangle problem

The first four eigenmodes will be solved with the MPM, and the subregions are defined with a 2 × 2 uniform coarse mesh. Fig. 2 shows the initial and final eigenfunction results, with the reference eigenfunctions as a comparison. For this test problem, there are no degenerated modes among the first four eigenmodes, and so all the modes converge stably as shown in Fig. 3.

4.2. 20 cm × 20 cm 2D square problem

4.2.1. The results without ARE

The first four eigenmodes will be solved with the MPM, and the subregions are defined with 2 × 2 uniform coarse meshes. For this test problem, the first and second eigenmodes are degenerated. The power operation matrix **A** is real symmetric, so its eigensolutions are all real, and the finally converged TM will also have only real eigensolutions. However, the TM is calculated using the integrals of the functions over the subregions, and the initialized functions are not symmetric, so the TM is not always symmetric during the simulation and it may have complex eigensolutions. If there are complex eigensolutions, all the eigenfunctions will not be updated by the MPM in this test without ARE.

The results are shown in Figs. 4 and 5. Fig. 4 shows that the final first and second eigenfunctions with the MPM are not the same as the reference, but they are the linear combination of the two reference modes. For this reason, the eigenvector errors are calculated with the normalized eigenvectors of two successive iterations, and they are shown in Fig. 5. The eigenvalue errors of the TM are also shown in Fig. 5, together with the imaginary parts of the eigenvalues of the TM. It can be seen that if there are complex eigenvalues of the TM, the convergence rate of the fundamental mode with the MPM is the same as the original power method. This is because the eigenfunction solutions are not updated by the MPM in this case, and so the first and second modes are not extracted from the fundamental mode. Once all the eigensolutions are real, the eigenfunction solutions can be updated, and so the eigensolution errors decrease dramatically. It is also confirmed in Fig. 5 that the imaginary parts of the eigenvalues are decreasing during the simulation and are much smaller than the real parts.

4.2.2. The results without BVF

For this test, the eigenvectors from the eigen-decomposition of the TM are directly used to update the functions without adopting the BVF. The results are shown in Fig. 6. It can be noticed that the eigenvectors of the first and second modes always fluctuate, while the convergence for the zeroth and third

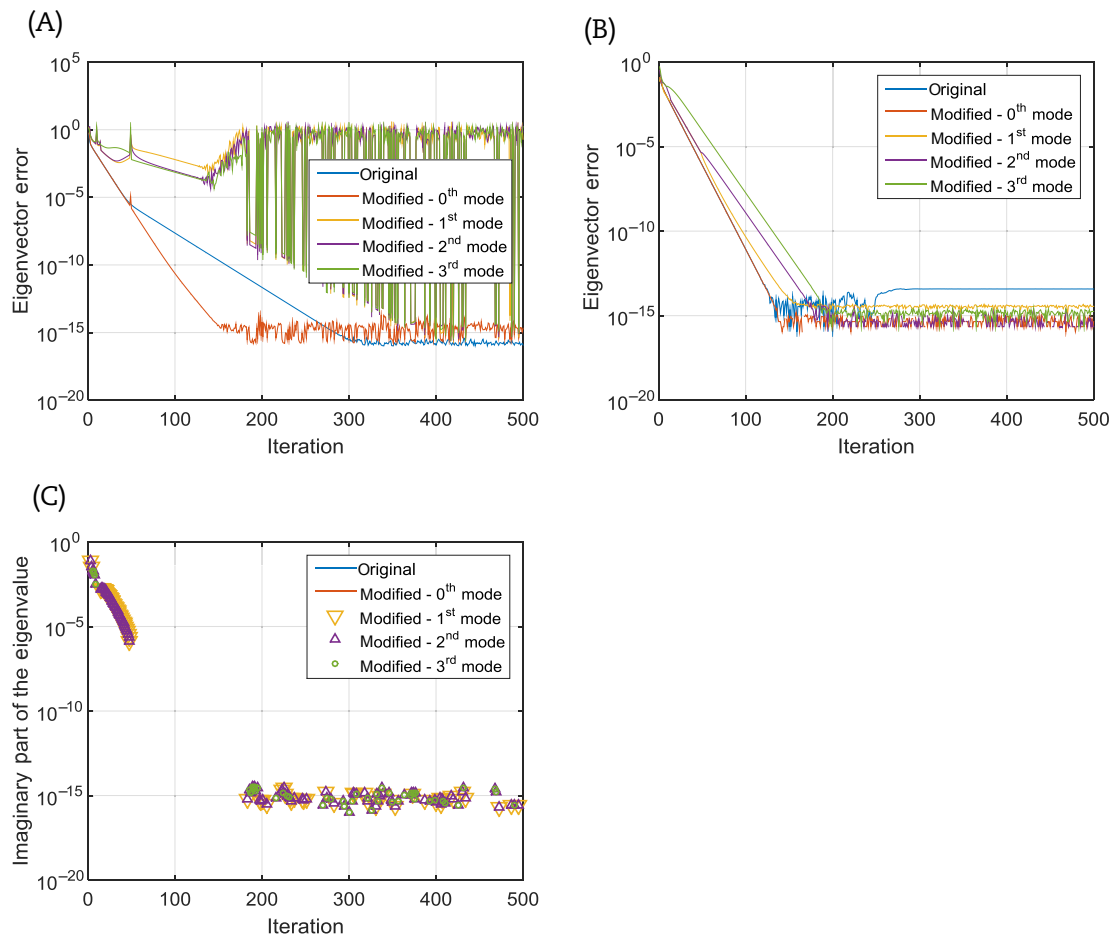


Fig. 8 – The results of the 3D cube without approximation to real eigenpairs. (A) The eigenvector errors; (B) eigenvalue errors; and (C) imaginary parts of the eigenvalues of the TM. TM, transfer matrix.

modes is stable. All the eigenvalues converge smoothly, since the eigenvalues have no relation with the eigenvectors' shape.

4.2.3. The results with both ARE and BVF

As shown in Fig. 7 for the eigenvector errors and the eigenvalue errors, all the eigensolutions converge stably if both ARE and BVF techniques are used.

4.3. 20 cm × 20 cm × 20 cm 3D cube problem

For the 2D square problem tested in the last section, the multiplicity of the degeneracy is 2. In order to test for multiplicity of > 2, a 3D cube problem is modeled, for which the multiplicity may be 3 or 6.

4.3.1. The results for the first four eigenmodes

The first four eigenmodes are solved with the MPM. The first, second, and third modes are degenerated. The results without ARE are shown in Fig. 8. Similar to the 2D square problem, if there are complex eigensolutions of the TM, all the functions are not updated, while they can be updated once all the eigensolutions of the TM are real, and the eigenvector errors decrease dramatically.

The results without BVF are shown in Fig. 9. Also similarly to before, the convergence of the zeroth mode is stable, while it is not stable for the degenerated modes, the first, second, and third modes.

The results with both techniques are shown in Fig. 10. All the eigenmodes converge stably.

4.3.2. The results for the first 20 eigenmodes

The first 20 eigenmodes are calculated using the MPM with both ARE and BVF techniques. The eigenvector and eigenvalue errors are shown in Fig. 11 and 12, respectively. It can be clearly observed that all the eigenmodes converge stably.

The first 20 eigenvalue results are listed in Table 2. The theoretical eigenvalues are also included for comparison, which are calculated according to the diffusion theory:

$$k_n = \frac{\nu \Sigma_f}{\Sigma_a + DB_g^2} = \frac{\nu \Sigma_f}{\Sigma_a + D \left(\frac{\pi}{a}\right)^2 (n_1^2 + n_2^2 + n_3^2)}, \quad n_1, n_2, n_3 = 1, 2, \dots \tag{17}$$

The eigenvalue spectrum is shown in Fig 13, which confirms that there is degeneracy with multiplicity of 3 and 6 for this 3D cube problem. In this case the techniques for dealing with the degenerated eigenmodes still work well.

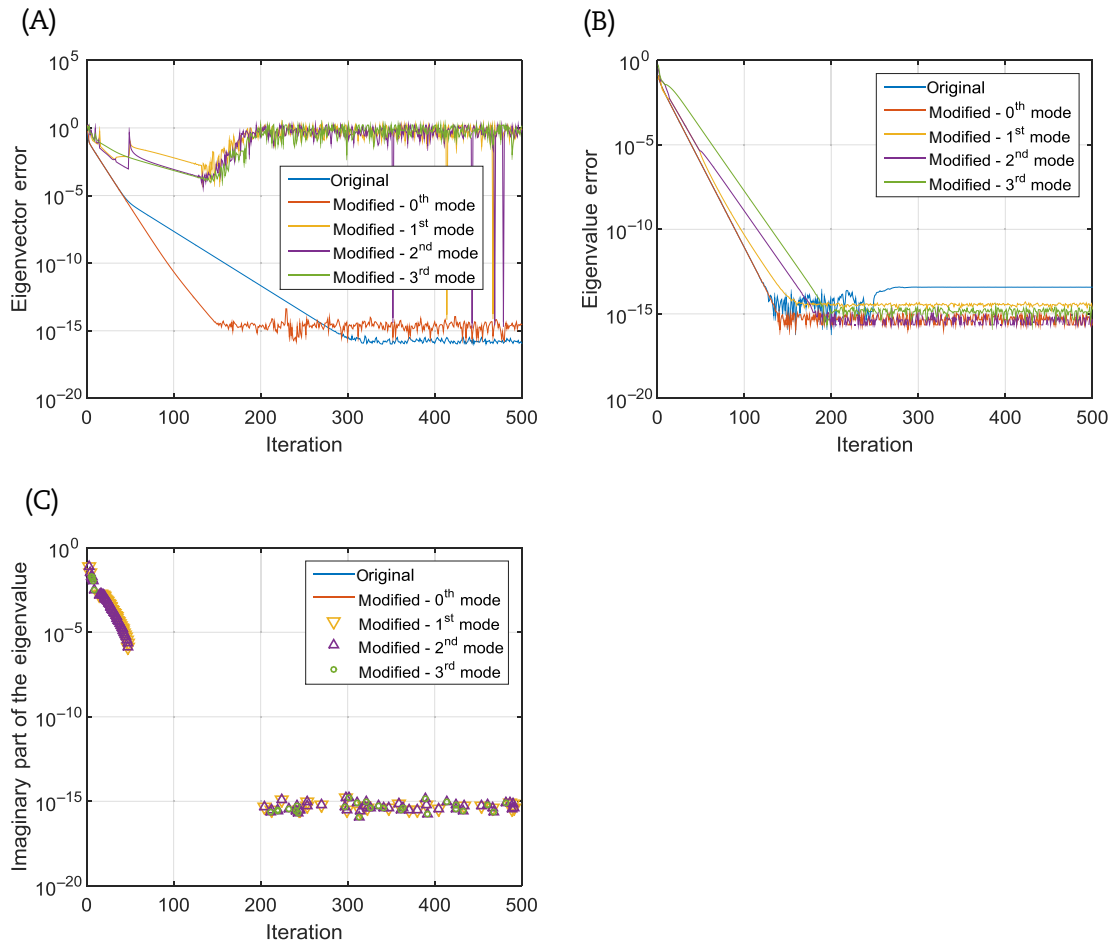


Fig. 9 – The results of the 3D cube without basis vector fixing. (A) The eigenvector errors; (B) eigenvalue errors; and (C) imaginary parts of the eigenvalues of the TM. TM, transfer matrix.

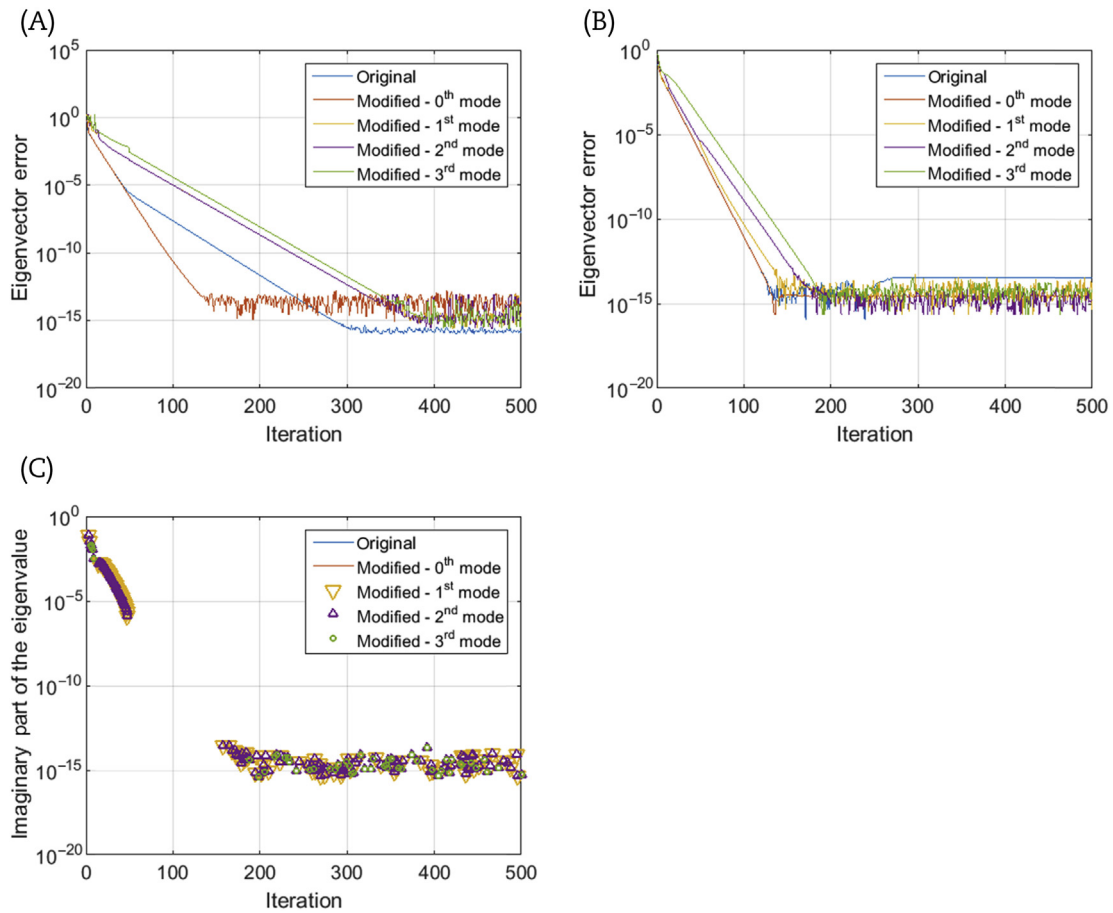


Fig. 10 – The results of the 3D cube with both approximation to real eigenpairs and basis vector fixing. (A) The eigenvector errors; (B) eigenvalue errors; and (C) imaginary parts of the eigenvalues of the TM. TM, transfer matrix.

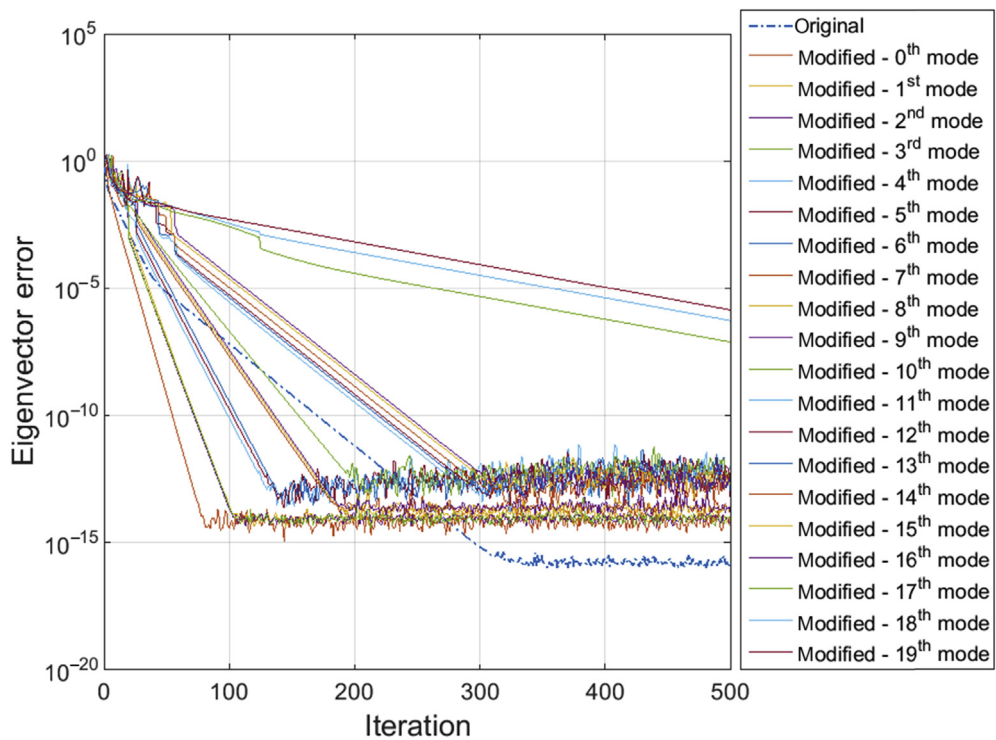


Fig. 11 – The eigenvector errors of the first 20 modes of the 3D cube problem.

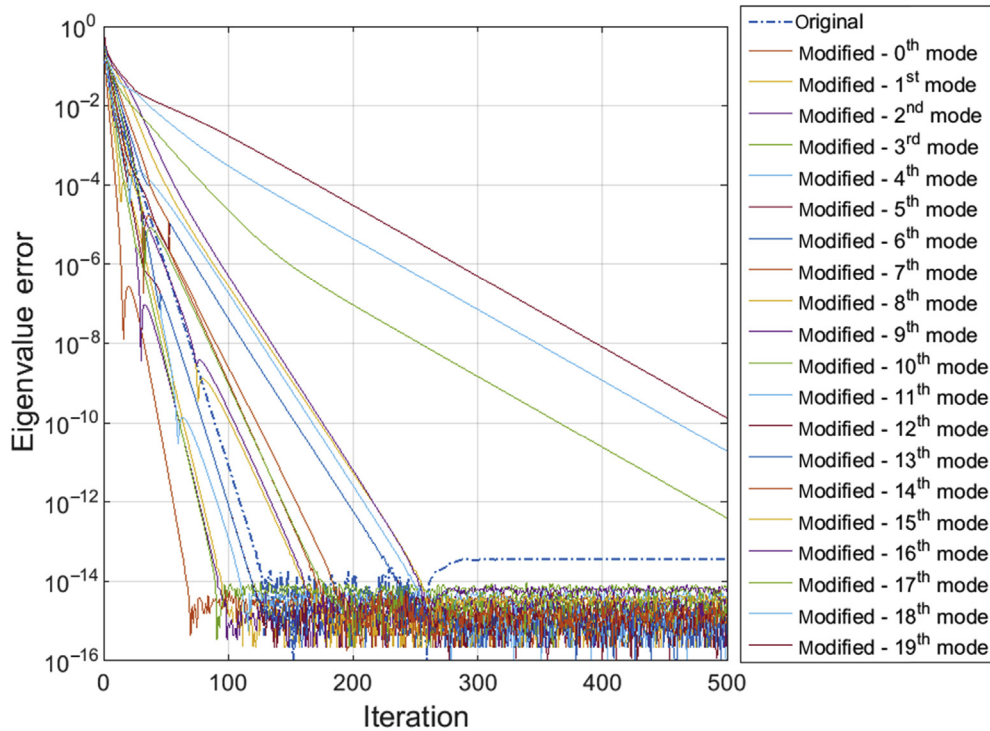


Fig. 12 – The eigenvalue errors of the first 20 modes of the 3D cube problem.

### 5. Conclusions

The application of the MPM to multidimensional problems may be unstable due to degeneracy issues. Complex intermediate eigenmode solutions are occasionally encountered in

such cases, and the shapes of the corresponding eigenvectors may change during the iterations. It is shown in this study that the imaginary components of the eigenvalues are much smaller than the real components, and the corresponding eigenvectors can be taken solely as the real and imaginary parts of the complex eigenvector solutions. In addition, the eigen-decomposition of the transfer matrix will give different eigenvectors for the degenerated eigenmodes every time, and a technique to fix the shapes of the degenerated eigenmodes is proposed by avoiding the combination of the corresponding modes when the eigenfunctions are updated.

Table 2 – The eigenvalue results of the 3D cube problem.				
Eigenvalue	Reference	Modified power method	(n1,n2,n3)	Diffusion theory
k0	1.354400	1.354400	(1,1,1)	1.354344
k1	1.234754	1.234754	(1,1,2)	1.234472
k2	1.234754	1.234754		
k3	1.234754	1.234754		
k4	1.134531	1.134531	(1,2,2)	1.134094
k5	1.134531	1.134531		
k6	1.134531	1.134531		
k7	1.076790	1.076790	(1,1,3)	1.075778
k8	1.076790	1.076790		
k9	1.076790	1.076790		
k10	1.049357	1.049357	(2,2,2)	1.048813
k11	0.999771	0.999771	(1,2,3)	0.998744
k12	0.999771	0.999771		
k13	0.999771	0.999771		
k14	0.999771	0.999771		
k15	0.999771	0.999771		
k16	0.999771	0.999771		
k17	0.933033	0.933033	(2,2,3)	0.932005
k18	0.933033	0.933033		
k19	0.933033	0.933033		

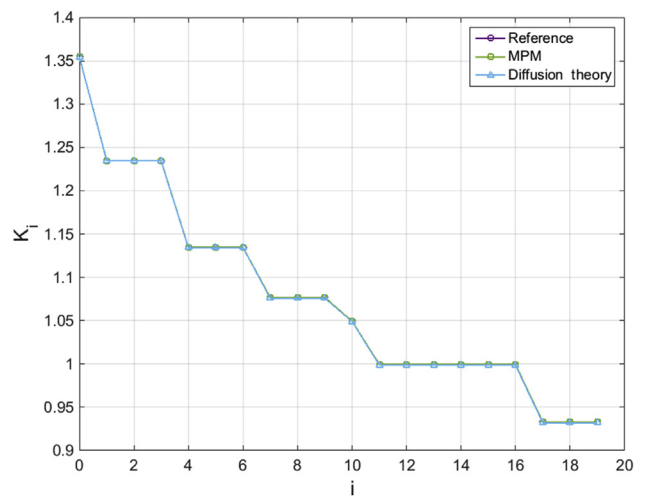


Fig. 13 – The eigenvalue spectrum of the 3D cube problem.

The performance of the techniques is demonstrated with two dimensional one group and three dimensional one group homogeneous diffusion problems. For more complicated problems, these techniques should also work well if similar degeneracy issues are encountered.

### Conflicts of interest

The authors have no conflicts of interest to declare.

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