Application of Modified Power Method to 2D Problems

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1. Introduction

The power method is commonly used for reactor criticality calculations, with which only the fundamental mode can be obtained, and the convergence ratio is determined by the dominance ratio k_l/k_0 . A modified power method was proposed recently [1-10], with which the first mode can be obtained and the convergence ratio can be k_2/k_0 . The authors extended the modified power method to get even higher modes, and the convergence ratio can be even smaller [11-13]. The application of this modified power method to 2D problems will be reported in this paper, and some problems that are different from 1D problems will be discussed.

2. The Modified Power Method

If starting with N initial sources, $\psi_1, \cdots \psi_N$, each of which can be thought as the linear combination of the targeted eigenfunctions, $\phi_1, \dots, \phi_N, \dots$, after one power iteration the sources can be updated as:

$$\psi_{i}' = A\psi_{i} = A\sum_{j} c_{ij}\phi_{j} = \sum_{j} c_{ij}k_{j}\phi_{j}, \ i = 1, \cdots, N,$$
 (1)

where A is the power iteration operator. After several power iterations, only the first N eigenmodes remain and the other higher modes can be neglected.

The idea of the modified power method is that the linear combination of these N sources will provide better estimators of the targeted first N eigenmodes:

$$(\psi_1 \quad \cdots \quad \psi_N) \begin{pmatrix} x_{11} & \cdots & x_{1N} \\ \vdots & \ddots & \vdots \\ x_{N1} & \cdots & x_{NN} \end{pmatrix} = (\psi_1' \quad \cdots \quad \psi_N'), (2)$$

where x_{ij} is the linear combination coefficient, and ψ_i ' provides a better estimator for ϕ_i .

In order to get the coefficients, N independent subregions are defined. Instead of estimating the eigenvalue by integrating over the whole system, it can be estimated by integrating over these local sub-regions, and all the local eigenvalue estimators should be equal. That is,

$$\begin{pmatrix} W_{11} & \dots & W_{1N} \\ \vdots & \ddots & \vdots \\ W_{N1} & \dots & W_{NN} \end{pmatrix} \begin{pmatrix} x_{11} & \dots & x_{1N} \\ \vdots & \ddots & \vdots \\ x_{N1} & \dots & x_{NN} \end{pmatrix} =$$

$$\begin{pmatrix} V_{11} & \dots & V_{1N} \\ \vdots & \ddots & \vdots \\ V_{N1} & \dots & V_{NN} \end{pmatrix} \begin{pmatrix} x_{11} & \dots & x_{1N} \\ \vdots & \ddots & \vdots \\ x_{N1} & \dots & x_{NN} \end{pmatrix} \begin{pmatrix} k_1 & \dots & 0 \\ \vdots & \ddots & \vdots \\ 0 & \dots & k_N \end{pmatrix},$$
(3)

where

$$W_{ij} = \int_{Rj} A\psi_i dr , \quad V_{ij} = \int_{Rj} \psi_i dr , \text{ and}$$

i = mode index, j = sub-region index.

Eq. (3) can be rewritten as

$$\mathbf{WX} = \mathbf{VXK},\tag{4}$$

and so

$$\mathbf{W} = \mathbf{V}\mathbf{X}\mathbf{K}\mathbf{X}^{-1} = (\mathbf{V}\mathbf{X})\mathbf{K}(\mathbf{V}\mathbf{X})^{-1}\mathbf{V} = \mathbf{F}\mathbf{K}\mathbf{F}^{-1}\mathbf{V} = \mathbf{P}\mathbf{V}, (5)$$

Once the integration terms W and V are obtained, the transfer matrix **P** can be calculated as:

$$\mathbf{P} = \mathbf{W}\mathbf{V}^{\cdot 1}.$$
 (6)

The Eigen decomposition of **P** will then provide the first N eigenvalues of the system which were contained in \mathbf{K} , and the sets of eigenvectors \mathbf{F} which can be used to solve the linear combination coefficients by:

$$\mathbf{X} = \mathbf{V}^{-1}\mathbf{F}.$$
 (7)

3. 2D Numerical Tests

3.1 Numerical test with finite difference method

A 2D square fuel slab problem was tested with finite difference method (FDM) in this part to show the capability of the modified power method to obtain higher mode solutions and accelerated convergence.

The size of the 2D slab is 10cm by 10cm, with the fuel cross sections listed in Table I. The mesh size is 0.1 cm for the calculations. For the modified power method, four eigenmodes were considered, and all the eigenmode fission sources were initialized as random numbers. The four sub-regions are divided by the centerlines of both directions.

The eigenvalue and eigenfunction results are shown in Table II and Fig. 1, respectively, in which the reference results are from the Eigen decomposition of the power matrix. Due to the symmetry of the problem, the 1st and 2nd modes have the same eigenvalue, and the eigenfunctions are not the same as the references, but the linear combinations of the references. The modified power method cannot distinguish the two modes. As shown in Fig. 2, the eigenvector errors of the two modes do not decrease, but fluctuate. For the 0th mode, the convergence is accelerated with the modified power method.

Table I. Fue	l Cross	Sections	for	FDM	Test

Σ_a (cm ⁻¹)	$v\Sigma_f$ (cm ⁻¹)	D (cm)
0.2	0.3	1/3

Table II. Eigenvalue Results

Eigenvalue	Reference	Modified Power Method
k_0	1.1287	1.1287
k_1	0.8232(0.73)	0.8232(0.73)
k_2	0.8232(0.73)	0.8232(0.73)
k_3	0.6478 (0.57)	0.6478 (0.57)



(a) Modified power method results.



(b) Reference results. Figure 1. The eigenfunction results.



Figure 2. The convergence error of different modes.

3.2 Numerical tests with MC

The modified power method was implemented in the Monte Carlo code MCS that was developed at UNIST [14]. The continuous energy cross section data are from the ENDF/B-VII.0 nuclear cross section library [15]. In order to perform the linear algebra operations, the precompiled Fortran 95 interface libraries BLAS95 and LAPACK95 contained in the Intel Math Kernel Library are adopted [16].

For the following 2D tests, four eigenmodes were considered. The four sub-regions were divided by the centerlines of both directions.

3.2.1 2D fuel slab with all black boundary conditions

The 2D fuel slab with black boundary conditions on four sides was modeled. The fuel composition is listed in Table III. In order to avoid the problem stated before with FDM, the size of the slab was set to be 40cm by 50cm. In this case the first several eigenvalues are different, as shown in Table IV. The reference case is one quarter of the slab with two reflective boundaries and simulated with the original power method. All the simulations were done with 100 inactive cycles, 500 active cycles, and 1,000,000 histories per cycle.

The initial and final converged eigenmode fission sources are shown in Fig. 4 and Fig. 5, respectively. The eigenmode solutions look reasonable, but the problem is that the Shannon Entropy values obtained with different methods are slightly different, as illustrated in Fig. 3. It cannot be concluded whether the modified power method is better or not, because the reference results obtained with the original power method may be not so reliable.

Table III. Fuel Composition

Concentration (#/barn-cm)			
7.6864e-05			
6.8303e-04			
5.9347e-02			
2.1220e-03			
3.7258e-02			

Method	Parameter	Value
Reference	k_0	1.01322 ± 0.00002
Original	k_0	1.01327 ± 0.00003
Modified Power Method	k_0	1.01324 ± 0.00003
	$k_1 (k_1 / k_0)$	$0.78192 \pm 0.00008 \ (0.772)$
	$k_2 (k_2/k_0)$	$0.69365 \pm 0.00009 \ (0.685)$
	$k_3 (k_3 / k_0)$	$0.55511 \pm 0.00011 \ (0.548)$



Figure 3. Shannon Entropy of 2D slab with black boundaries.



Figure 4. The initial fission sources.



Figure 5. The converged fission sources.

3.2.2 2D fuel slab with all reflective boundaries

The 2D fuel slab problem with the same size and fuel composition as before was modeled, but with reflective boundaries on four sides. Theoretically, for this case the 0^{th} eigenfunction should be flat. All the simulations were done with 100 inactive cycles, 500 active cycles, and 1,000,000 histories per cycle.

Table V. Eigenvalue Results			
Method	Parameter	Value	
Original	k_0	1.29521 ± 0.00001	
Modified Power Method	k_0	1.29524 ± 0.00001	
	$k_1 (k_1 / k_0)$	$1.14429 \pm 0.00007 (0.883)$	
	$k_2 (k_2/k_0)$	$1.07284 \pm 0.00007 \ (0.828)$	
	$k_3 (k_3 / k_0)$	$0.96311 \pm 0.00009 (0.744)$	



Figure 6. The initial fission sources.



Figure 7. The converged fission sources.



Figure 8. Shannon Entropy of 2D slab with reflective boundaries.

The simulated eigenpair results are shown in Table V and Fig. 7. The initial 0th mode fission source was set to be just in one quarter of the slab, as shown in Fig. 6. Fig. 8 shows that the Shannon Entropy value of the modified power method is slightly lower than the theoretical value that is estimated with flat distribution, but much closer to it than the original power method. If 10 times of histories per cycle was adopted for the original power method, the Shannon Entropy value would be similar to the modified power method, as shown in Fig. 8.

3.2.3 PWR Assembly problem

This test is to show the performance of the modified power method for more practical problems. A 2D PWR assembly with 17 by 17 fuel rod lattice is modeled, with reflective boundaries on 4 sides. No guide thimbles for the control rods and the movable detectors are modeled. The main geometry and material parameters of the pin cell are listed in Table VI. All the simulations were done with 30 inactive cycles, 90 active cycles, and 100,000 histories per cycle.

Parameter	Value
Radius of fuel pellet, cm	0.392180
Inner radius of the cladding, cm	0.400050
Outer radius of the cladding, cm	0.457200
Fuel pin pitch, cm	1.259840
Fuel type	1.6 enriched UO ₂
Cladding type	Zircaloy 4
Coolant density, g/cm^3	0.740582
Boron concentration, ppm	976

Table VII. Eigenvalue Results

Method	Parameter	Value
Reference	k_0	1.02982 ± 0.00019
Original	k_0	1.02973 ± 0.00017
	k_0	1.02998 ± 0.00017
Modified	$k_1 (k_1 / k_0)$	0.40289±0.00107 (0.391)
Method	$k_2 (k_2/k_0)$	0.40268±0.00107 (0.391)
	$k_3 (k_3 / k_0)$	0.21025±0.00201 (0.204)



Figure 9. The initial fission sources.



Figure 10. The converged fission sources.

The simulated eigenvalues are shown in Table VII. The reference is from the simulation of one pin cell of the same type with original power method. The fundamental eigenvalues of different simulations are consistent. It is worthy noticing that the Dominance Ratio (k_1/k_0) of this assembly is about 0.4.

The initial and converged fission sources are shown in Fig. 9 and Fig. 10. Due to the symmetry of the assembly, the 1^{st} and 2^{nd} modes have the same eigenvalue, so they cannot be distinguished by the modified power method. The converged fission sources of the 1^{st} and 2^{nd} modes may be affected by the initial values, but it is not clear now. However, this will not affect the other eigenmode results.

As shown in Fig. 11(1), the Shannon Entropy of the modified power method is higher than the original power method and closer to the theoretical value. The Root Mean Square Error (RMSE) of the fundamental mode is then compared, which can be calculated with:

$$RMSE = \sqrt{\frac{1}{N_{mesh}} \sum_{n=1}^{N_{mesh}} \left(\phi_n - \phi_{n,ref}\right)^2},$$
 (6)

where

$$\phi_{n,ref} = 1/289$$

As shown in Fig. 11(2), the RMSE of the modified power method is lower, which means that the modified power method outperforms the original power method by producing a more accurate result.



4. Conclusions

The application of the modified power method to 2D problems is studied. It can be concluded that the modified power method can be applied to practical problems like PWR assembly calculations. The performance of the modified power method is better than the original power method, not only for the accelerated fission source convergence, but also for the better fundamental fission source distribution. The modified power method can't distinguish the eigenmodes if they have the same eigenvalue, but this will not affect the other mode solutions. More work needs to be done to automate the initialization of fission sources and to investigate the effects of sub-region definitions.

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