Automated Determination of Optimum Subspace Dimension in Krylov Depletion Method

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1. Introduction

The Kylov subspace method calculation of matrix exponentials has been used for fast, yet accurate depletion calculations.[1,2] Although the accuracy of this method depends on the dimension of the Krylov subspace which should be problem dependent, a predetermined fixed dimension is used in most existing codes. The use of excessively high subspace dimension imposes a significant calculation burden without increasing much the accuracy while too small subspace dimension can deteriorate the solution. Therefore there is a need for determining the proper dimension size which would satisfy the competing requirements of accuracy and speed.

In this study, an automated Krylov subspace expansion is introduced in order to solve the problem of fixing the subspace dimension in advance. The background of the Krylov subspace based depletion is explained first, and then the results of the automated Krylov subspace expansion are presented below.

2. Methods and Results

The essence of the Krylov subspace based depletion method is to expand the matrix exponential involved in the solution of the depletion equation. The expansion is done in gradually increasing subspaces which can be optimally determined by the methods explained below.

2.1 Krylov Subspace Expansion of Matrix Exponential

The general solution for the depletion equation can be written as:

$$\boldsymbol{N}(t+\Delta t)=e^{\mathbf{A}\Delta t}\boldsymbol{N}(t) \tag{1}$$

where $\boldsymbol{N}$, $\boldsymbol{A}$ and Δt are the nuclide vector, depletion matrix, and the depletion time step size, respectively. By introducing the Krylov subspace method, the solution of the above equation can be written as:

$$\boldsymbol{N}(t+\Delta t)\approx\beta\ \boldsymbol{V}_m\ e^{\boldsymbol{H}_m\Delta t}\ \boldsymbol{e}_1 \tag{2}$$

where

$\beta=\left\|\mathbf{N}(t)\right\|_2$

$\boldsymbol{V}_m=[\boldsymbol{v}_1,\boldsymbol{v}_2,\cdots,\boldsymbol{v}_m]$

$\boldsymbol{H}_m$ Hessenberg (upper triangular with an extra sub-diagonal) matrix, and

$\boldsymbol{e}_1=[1,0,\cdots,0]^T$.

By this, the depletion matrix which has a large size (more precisely, dimension) is transformed into a small size Hessenberg matrix. The size of the Hessenberg matrix is determined by the dimension of the Krylov subspace employed.

2.2 Characteristic of Hessenberg matrix elements

Fig.1 shows the process of generating the new orthogonal basis vector from known orthogonal basis vectors. In this process, the effect of the new vector $A\vec{v}_j$ is determined by the size of its projection to the new orthogonal basis vector, namely, $h_{j+1,i}$. If the new orthogonal component of $A\vec{v}_j$ is small, it can be considered negligible in constructing the next dimension Krylov subspace.

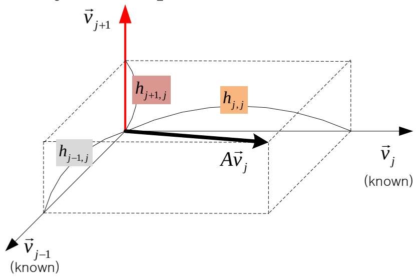

Fig. 1. Process of generating new orthogonal basis

This concept can also be found in the relation between a depletion matrix and a Hessenberg matrix which can be written as:

$$\boldsymbol{AV}_m=\boldsymbol{V}_m\boldsymbol{H}_m+h_{m+1,m}\boldsymbol{v}_{m+1}\boldsymbol{e}_m^T \tag{3}$$

where

$h_{m+1,m}$ = the last entry in the Hessenberg matrix.

Here if the size of the last entry in the Hessenberg matrix is neglected, the following approximation can be possible:

$$\boldsymbol{AV}_m\simeq\boldsymbol{V}_m\boldsymbol{H}_m \tag{4}$$

That is to say, the depletion matrix can be approximated without further orthogonal basis vectors.

2.3 Automated Control of Krylov subspace dimension

Let us examine the relation between the size of $h_{m+1,m}$ and the error of solutions versus Krylov subspace dimension. Using a depletion matrix generated during a UO_2 depletion, the results shown Fig. 2 can be obtained which reveals that the size of $h_{m+1,m}$ is gradually decreasing like the solution error although it is fluctuating. Thus there is a possibility of controlling the Krylov subspace dimension using $h_{m+1,m}$.

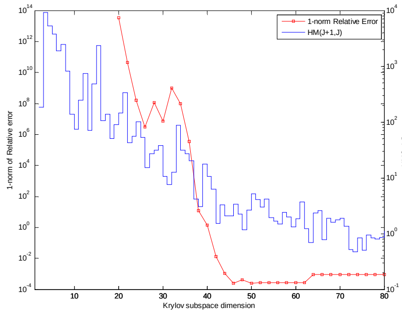

Fig. 2. Last entry of Hessenberg matrix and solution error versus Krylov subspace dimension

In order to realize this idea, a criterion is needed to determinine the cut-off value of $h_{m+1,m}$. However it is difficult to determine the criterion due to the fluctuation behavior of $h_{m+1,m}$. To resolve this problem, the least squares method is introduced here. The following fitting function is taken

$$h(m) = \frac{1}{am+b} \qquad (5)$$

Considering the decreasing behavior of $h_{m+1,m}$ with *m*. Previous 20 points are used in the least square fitting. As the result of the least square fitting, the fluctuation of $h_{m+1,m}$ can be smoothened as shown in Fig. 3. Now it is be possible to determine stably the termination point of Krylov subspace expansion, for example 10 for the size of $h_{m+1,m}$ in Fig. 3.

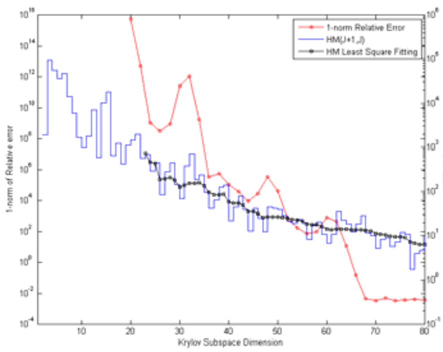

Fig. 3. Least square fitting of $h_{m+1,m}$

2.4 Performance Examination

The automated Krylov subspace expansion was implemented in the nTRACER direct whole core calculation code[3] and a UO_2-Gd pin cell checkerboard was solved to examine the effectiveness the proposed automated scheme. Fig. 4 shows the results of the test calculation. In the left figure of Fig. 4 which shows the k-eff vs. burnup behavior, it is observed that there is essentially no difference between the k-eff's of case of automated dimension and the case of a fixed dimension of 80. The right figure showing the automatically determined dimensions for each fuel type indicates that more dimensions are used in Gd cell than UO_2 and those are far less than 80 for both. This demonstrates clearly the fact that the proper Krylov subspace dimension should be dependent on the characteristics of the problem, mainly, composition. As shown in Table I, the computing time for depletion can be significantly reduced by a factor of 3.

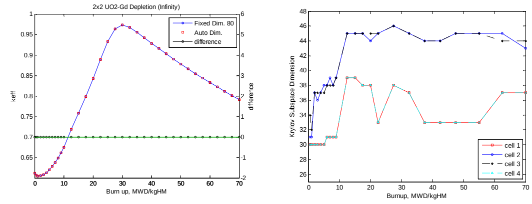

Fig. 4. Depletion result with the automated scheme

Table I: Comparison of depletion calculation time, sec

Fixed dimension (80)	Automated Krylov subspace expansion
30.6	9.6

3. Conclusions

In order to solve the problem of using predetermined fixed subspace dimension in the Krylov subspace based depletion method, the behavior of the size of the new subspace component was examined and an automated control scheme of Krylov subspace dimension was developed which is based on a least square fitting of the last entry of the Hessenberg matrix. This scheme determines autonomously the proper dimension according to the degree of problem difficulty. It was shown that fast and accurate subspace expansion was possible with the proposed scheme. This automated method has two advantages, namely, the autonomous determination of the optimum dimension according to the problem characteristics and the significant reduction in the computing time for depletion calculations.

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