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Krylov-Schur 순환법에 의한 2차원 사각도파관에서의 고유치 문제에 관한 연구

(A Study On The Eigen-properties of A 2-D Square Waveguide by the Krylov-Schur Iteration Method)

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요 약

Krylov-Schur 반복법을 활용하여 2-차원 사각 도파관에서 나타나는 고유특성을 밝혔다. 고유 행렬 방정식은 삼각형 그물 요소의 접선을 기저벡터로 사용한 FEM(유한요소법)으로 구성하였다. 우선 Arnoldi 분해법을 이용하여 이 방정식에 대한 상위 Hessenberg 행렬을 구하였다. 그리고 QR 알골리즘을 통하여 이것을 삼각형 대각 행렬인 Shur 형태로 변형하였다. 수렴 조건에 부합된 몇몇 고유 값들이 삼각형 대각 행렬의 대각 요소에 나타났다. 이들에 대응하는 고유 모드들을 역-반복법으로 구하였다. 수렴조건에 부합되는 고유 값들은 Shur 행렬의 대각선 선두 부분으로 재배열시켰다. 이들은 나머지 고유값 및 고유모드의 쌍을 구하는 반복 과정에서 변형되지 않도록 배제되었다. 이 과정이 연속하여 서너 번 반복되었는데, 그 결과 충분한 신뢰도를 갖는 주요한 몇 개의 TM 및 TE 고유 쌍들이 구하여졌다.

Abstract

The Krylov-Schur algorithm has been applied to reveal the eigen-properties of the wave guide having the square cross section. The eigen-matrix equation has been constructed from FEM with the basis function of the tangential edge-vectors of the triangular element. This equation has been treated firstly with Arnoldi decomposition to obtain a upper Hessenberg matrix. The QR algorithm has been carried out to transform it into Schur form. The several eigen values satisfying the convergent condition have appeared in the diagonal components. The eigen-modes for them have been calculated from the inverse iteration method. The wanted eigen-pairs have been reordered in the leading principle sub-matrix of the Schur matrix. This sub-matrix has been deflated from the eigen-matrix equation for the subsequent search of other eigen-pairs. These processes have been conducted several times repeatedly. As a result, a few primary eigen-pairs of TE and TM modes have been obtained with sufficient reliability.

Keywords: FEM, Krylov-Schur method, Arnoldi decomposition, QR algorithm, inverse iteration metho

Ⅰ. INTRODUCTION

The eigen-problem describing the hypothetically infinite long waveguide has been solved by upper triangulating the matrix equation resulted from FEM (Finite Element Method). It has been assumed that the cross sectional area of the waveguide is a square form and its surface is coated with perfect conductor.

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It has been also assumed that the inner space of the waveguide is emptied or filled with linear and homogeneous material. The structural properties impose a translational symmetry on the waveguide along the axial direction. The conductor coated on the surface makes the problem an easy task by confining the electromagnetic field just in the waveguide without any leakage. So, it is possible that the eigen-properties of waveguide can be characterized just in the 2-dimensional plane crossing it perpendicularly.

The space of the waveguide has been divided into the elemental domains of the structured triangles. These triangles have been the same form but, systemically overlapped with each other only through the common edges to fill the entire space. The basis function has been chosen based on the tangential edge vectors of the triangular element. It has been well known that this choice would promise the continuity of the tangential electric and magnetic field strength over the interface and surface. It would also be expected to eliminate the possibility of spurious corruption in the numerical calculation[1]. FEM has been carried out using the Galerkin method of weighted residuals to construct the linear equation[2]. As a result, the matrices have been the symmetrically banded form and the eigen-matrix equation has been assembled from them.

If dimension of the matrices forming this equation is small, the eigen-values and eigen-modes will be easily obtained through the bulge chase QR-decomposition[3]. However, to fulfill a more confidential calculation, it is required that the elemental meshes must be more divided precisely and refined finely. This process would be accompanied by increasing the dimension of the matrices and unknown parameters. The larger dimension makes the calculation more difficult, because of the heavy memory demanding and the slowly converging rate in the upper triangulating process. These reasons would diminish the efficiency of this iterative QR-decomposition method. To overcome these difficulties, iterative restating algorithms have been introduced continuously since 1990 and applied successfully to various eigen-problems. Among these, the G. W. Stewart's Krylov-Schur iteration method has been recognized as the most brilliant algorithm[4~5]. It has been well known that this algorithm would generate the satisfactory results for the eigen-matrix equation even if it was composited with non-symmetric matrices.

The main object in this study has been to clearly reveal the eigen-properties of the TE(Transverse Electric) and TM(Transverse Magnetic) modes through iterative restarting Krylov-Schur algorithm. In the last few decades, there have been many similar researches on this purpose with other various algorithms[6~7]. And by these unwearying strives, several algorithms have been settled down and employed to resolve the difficult problems in the application fields. Nevertheless, it may be reasonable to make a more affirmation on the Krylov-Schur algorithm to solve the general eigen-problems for the development of the numerical analysis techniques.

II. FINITE ELEMENT FORMULATION

The propagating transverse waves in a homogeneous waveguide are divided into TE and TM modes. These transverse waves satisfy the vector Helmholtz equation of the dual form

$$\overrightarrow{\nabla}_t \times \left(\frac{1}{\nu}\overrightarrow{\nabla}_t \times \overrightarrow{F_t}\right) - k^2\zeta\overrightarrow{F_t} = 0 \qquad (1)$$

where $k=\omega\sqrt{\epsilon_0\mu_0}$ is the propagation wave number and, for the TE mode $\overrightarrow{F_t}=\overrightarrow{E_t}$ (transverse electric field strength), $\nu=\mu_r$(relative permeability μ/μ_0), $\zeta=\epsilon_r$ (relative ppermittivity ϵ/ϵ_0) and, for the TM mode $\overrightarrow{F_t}=\overrightarrow{H_t}$ (transverse magnetic field strength),$\nu=\epsilon_r$, $\zeta=\mu_r$. From inner producting the eq.(1) with a testing vector function T_t and integrating over the area of the waveguide, it can be written as

$$\iint_{\Omega} \overrightarrow{T_t} \cdot [\overrightarrow{\nabla_t} \times (\frac{1}{\nu}\overrightarrow{\nabla_t} \times \overrightarrow{F_t}) - k^2\zeta\overrightarrow{F_t}]ds \qquad (2)$$

The first term can be expanded from the vector identity of the divergence theorem as following

$$\begin{aligned}&\iint_{\Omega} \overrightarrow{T_t} \cdot \overrightarrow{\nabla_t} \times (\frac{1}{\nu}\overrightarrow{\nabla_t} \times \overrightarrow{F_t})ds \\ &= \iint_{\Omega} (\overrightarrow{\nabla_t} \times \overrightarrow{T_t}) \cdot (\overrightarrow{\nabla_t} \times \overrightarrow{F_t})ds \\ &\quad - \oint_{r} \hat{n} \cdot [\overrightarrow{T_t} \times (\frac{1}{\nu}\overrightarrow{\nabla_t} \times \overrightarrow{F_t})]dl\end{aligned} \qquad (3)$$

The waves must satisfy the boundary condition on the surface coated with perfect conductor. For TE mode, the vector testing function T_t is set to zero in order to satisfy the Dirichlet boundary condition. For the TM mode, the normal derivative value $\frac{1}{\nu}\overrightarrow{\nabla_t} \times \overrightarrow{F_t}$ is assumed to be zero to meet with the Neumann boundary condition. By these reasons, the contour integral can be omitted from the eq.(3). As a result, the equation describing the propagating waves can be written as

$$\begin{aligned}&\iint_{\Omega} (\overrightarrow{\nabla_t} \times \overrightarrow{T_t}) \cdot (\overrightarrow{\nabla_t} \times \overrightarrow{F_t})ds \\ &\quad - \iint_{\Omega} k^2\zeta\overrightarrow{F_t}ds = 0\end{aligned} \qquad (4)$$

To proceed the numerical analysis without spurious corruption, the vector basis function of the triangular element is constructed by employing the constant tangential edge vectors. The vector basis function is related with these edge vectors through the barycentric coordinates[8~9]. The triangular element and the corresponding notations are shown in the Fig.1(a). From this figure, the 2-dimensional barycentric coordinates $(\mathcal{L}_1, \mathcal{L}_2, \mathcal{L}_3)$ corresponding to the position $\vec{r} = x\overrightarrow{e_x} + y\overrightarrow{e_y}$ in the element area can be related to the vertex positions $\overrightarrow{r_i} = x_i\overrightarrow{e_x} + y_i\overrightarrow{e_y}$, $i = 1,2,3$ and the centroidal position $\overrightarrow{r_c} = \frac{1}{3}(\overrightarrow{r_1} + \overrightarrow{r_2} + \overrightarrow{r_3})$ of the triangular element as following

$$\mathcal{L}_i(\vec{r}) = \frac{A_i}{A} = \frac{1}{3} - (\vec{r} - \overrightarrow{r_c}) \cdot \frac{\overrightarrow{r_{jk}} \times \overrightarrow{e_z}}{J} \qquad (5)$$

where J is the so called Jacobi determinant of the matrix $[A] = \begin{pmatrix} 1 & 1 & 1 \\ x_1 & x_2 & x_3 \\ y_1 & y_2 & y_3 \end{pmatrix}$ having the relation $A = \frac{J}{2}$ with the area A of the triangular element. The value of A_i is the area of the triangle of the vertices P, k, j. From this relation, it is identified that the barycentric coordinates can be represented with the production between 3×3 and 3×1 matrices as like the linear shape functions of the triangular element

$$\begin{pmatrix} \mathcal{L}_1 \\ \mathcal{L}_2 \\ \mathcal{L}_3 \end{pmatrix} = \frac{1}{2A}\begin{pmatrix} a_1 & b_1 & c_1 \\ a_2 & b_2 & c_2 \\ a_3 & b_3 & c_3 \end{pmatrix}\begin{pmatrix} 1 \\ x \\ y \end{pmatrix} \qquad (6)$$

where

$$a_i = x_j y_k - x_k y_j,\ b_i = y_j - y_k,\ c_j = x_k - x_j$$

$(i, j, k$ are cyclic ordered vertex indexes) are the components of the un-normalized inverse matrix $[A]^{-1}$. With these barycentric coordinates, the tangential edge vectors $\overrightarrow{W_{ti}}$ are constructed as following

$$\overrightarrow{W_{ti}} = l_i(\mathcal{L}_j\overrightarrow{\nabla_t}\mathcal{L}_k - \mathcal{L}_k\overrightarrow{\nabla_t}\mathcal{L}_j) \qquad (7)$$

where l_i is a length of the edge numbered i, and i, j, k are indexes of the barycentric coordinates in cyclic ordering. Using these tangential edge vectors, the field strength in the single triangular element can be represented as following

$$\overrightarrow{F_t} = \sum_{i=1}^{i=3} e_{ti}\overrightarrow{W_{ti}} \qquad (8)$$

where e_{ti} is to be found i-th unknown edge field depicted in the Fig.1(b). As can be seen from this figure, a triangle and its neighbors are arranged in the opposite directions with respect to each other. This is the reason for consistently defining the direction of the edge vector. Substituting the eq.(8) for $\overrightarrow{F_t}$ and replacing $\overrightarrow{T_t}$ with $\overrightarrow{F_{tj}}$ in the eq.(4), this equation can be rewritten as following

$$\frac{1}{\nu}\sum_{i=1}^{i=3}\iint_A (\overrightarrow{\nabla_t}\times\overrightarrow{W_{tj}})\cdot(\overrightarrow{\nabla_t}\times\overrightarrow{W_{tj}})e_{ti}ds - k^2\zeta\sum_{i=1}^{i=3}\iint_A (\overrightarrow{W_{tj}}\cdot\overrightarrow{W_{tj}})e_{ti}ds = 0 \tag{9}$$

where subscript A indicates the integration over the triangular element. This equation can be rearranged into a matrix form

$$[S_{el}]\{e_t\} = k^2[T_{el}]\{e_t\} \tag{10}$$

where

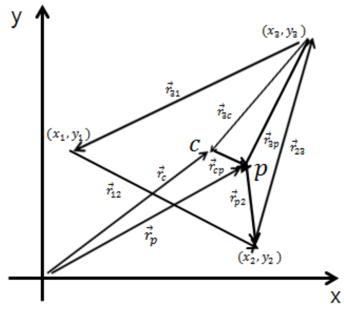
$[S_{el}] = \frac{1}{\nu}\iint_A (\overrightarrow{\nabla_t}\times\overrightarrow{W_{tj}})\cdot(\overrightarrow{\nabla_t}\times\overrightarrow{W_{ti}})ds$ and $[T_{el}] = \zeta\iint_A (\overrightarrow{W_{tj}}\cdot\overrightarrow{W_{ti}})ds$. These element matrix equations can be assembled over all triangular meshes of the waveguide to obtain a global eigen-matrix equation.

$$[S]\{e_t\} = k^2[T]\{e_t\} \tag{11}$$

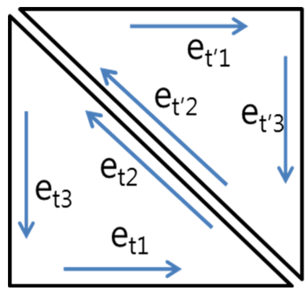
In this equation, $[S]$ and $[T]$ are a $n\times n$ square matrices and $\{e_t\}$ is a $n\times 1$ column matrix where n is a total number of the edges composing the mesh of the waveguide. When obtaining the eigen-pairs of the TE mode, the tangential components of the electric fields must satisfy the Dirichlet boundary condition. This is accomplished in implementing the programs by cancelling the edge components of the triangular elements which coincide with the wall of the waveguide.

Ⅲ. KRYLOV-SCHUR ITERATION METHODE

Usually, the dimension of the eigen-matrix equation resulting from FEM is too large to obtain all the eigen-modes at one time. In practice, however it



(a) 요소와 무게중심좌표
(a) The mesh and barycentric coordinate



(b) 요소의 접선 모서리 벡터
(b) The tangential edge vectors

그림 1. 요소 삼각형의 배열 개요
Fig. 1. The schematic representation of the element triangular mesh and its arrangement.

is interested only in finding the few eigen-pairs. So, in this study, it has been strived to obtain a few prominent eigen-pairs corresponding to the smallest eigen-values. It has been well known that the Krylov-Schur iteration method is the one of most reliable technique for finding the prominent eigen-pairs.

V. Hernändez et al., have summarized the essence of this algorithm in the compact form as following[10].

[Krylov-Schur method]
Input: Matrix $[M]$ and initial vector $\{\nu_1\}$ with number of the decomposition dimension m.
Output: $c \le m$ Ritz pairs.
1. Build a Hessenberg matrix of order m by Arnoldi decomposition.
2. Apply QR algorithm to get a Schur matrix.
3. Fine the eigen-pairs by inverse iteration method.

4. If there are w eigen-pairs satisfying the pre-determined condition, reorder them to first primary diagonal block through unitary similarity transform.
5. if $w < c$, truncate the resulting Schur matrix at position w and go to step 1.
6. Extend the matrix with the residual vector $\tilde{v} = \tilde{v}_{w+1}$ as a initial vector by Arnoldi decomposition.

To apply this method, it is convenient to transform the eq.(11) by the shift-invert strategy previously as following

$$\frac{1}{k_c^2 - \sigma}\{e_t\} = \frac{[T]}{[S] - \sigma[T]}\{e_t\} = [M]\{e_t\} \qquad (12)$$

Because of the dependence on the shift value σ, it is expected that the convergence rate will be more promoted at this value than anything else. In step 1, the Arnoldi decomposition of order m is performed on the matrix $[M]$. It computes an orthogonal basis V_m in the Krylov subspace and at the same time obtains the projected Hessenberg matrix $[H_m]$

$$[M][V_m] = [V_m \ V_{m+1}]\begin{bmatrix} H_m \\ \\ b_{m+1}^{*} \end{bmatrix} \qquad (13)$$

where $[V_m]$ and $[H_m]$ has a dimension $n \times m$ and $m \times m$ respectively. A Gram-Schmidt procedure carried out to make the Arnoldi vectors orthogonal with respect to each other and to remove all other components from them[11]. The vectors $\{b_{m+1}\}$ are the residual vectors which involve the information to appraise the accuracy of the Ritz values resulted from the Arnoldi algorithm. For step 2, QR algorithm is applied to this Hessenberg matrix to transform it into the real Schur form $[T_m]$[12]. This algorithm is established with an orthogonal matrix$[Q_1]$ which transforms the matrix H_m such as $[T_m] = [Q_1^{*}][H_m][Q_1]$. . The Ritz values are deduced from the 1×1 or 2×2 diagonal blocks of this quasi upper triangular matrix. The eigen-values λ_w and eigen-modes ϕ_w for the Schur matrix are calculated from the inverse iteration method by the matrix $[Q_2]$ [13]. Among these, the wanted eigen-pairs are selected out from the relations

$$\begin{aligned} &\| [M]([V_m][\phi_w]) - \lambda([V_m][\phi_w]) \|_2 \\ &\quad = \left| \left\{ b_{m+1}^T \right\} \{\phi_w\} \right| \\ &\quad\ \le \max\left\{ u \| T_m \|_F, Tol \times \lambda_w \right\} \end{aligned} \qquad (14)$$

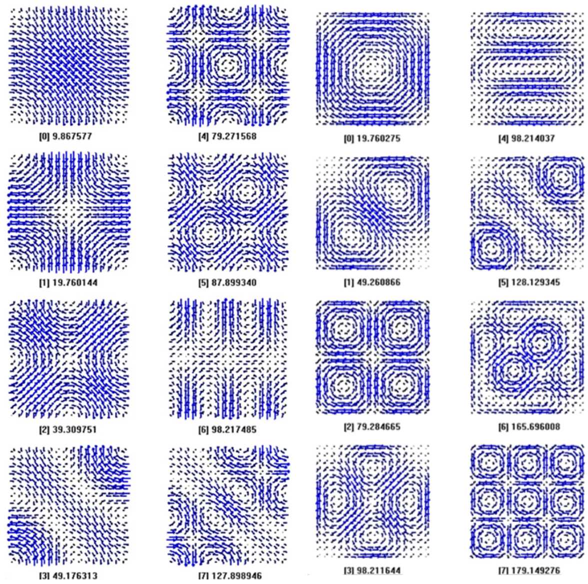
where u and $\| * \|_F$ are the unit round off and the Frobenius norm respectively, and Tol is an arbitrary defined tolerant value. As initial results, there are some eigen-pairs satisfying the above convergent condition. These values are referred to as wanted eigen-values which may be usually located in various parts of the spectrum. These wanted eigen-pairs should be reordered to the leading principle sub-matrix $[T_w]$, because these pairs no longer participate in the subsequent search for other eigen-pairs. This can be accomplished by means of unitary similarities with transforming matrix $[Q_3]$ in step 4[14]. The deflation is conducted by truncating the matrices at the index w from the step 5. The next Arnoldi decomposition is carried out with the equation $[M][\widehat{V_w}] = [\widehat{V_w}, \tilde{v}]\begin{bmatrix} T_w \\ \\ \tilde{b}_w \end{bmatrix}$ by locking the sub-matrix $[T_w]$ without any disturbance. By deflation, it may be expected that decompositing operations in Arnoldi cycles may be alleviated and improved. In step 6, the subsequent Arnoldi decomposition is extended over this equation to the remaining components. The Arnoldi vectors are computed with the initial vector $\tilde{v} = \widetilde{v_{w+1}}$ of the result relation $[\widetilde{V_m}] = [V_m][Q_1][Q_2][Q_3]$, but $\tilde{v}_1$ to $\tilde{v}_w$ of them are also taken into account in orthogonalization processes. As a result, the following equation is obtained by repeatedly applying the above mentioned upper diagonalizing and exchanging processes to the result of the Arnoldi decomposition,

$$
\begin{aligned}
&[M][\widehat{V_w}, \tilde{v}, \widetilde{V_{m-w-1}}] \\
&= [\widehat{V_w}, \tilde{v}, \widetilde{V_{m-w}}]\begin{pmatrix} T_w & * & * \\ & \lambda_{w+1} & * \\ & & \widetilde{B_{m-w-1}} \\ & \widetilde{b_{w+1}} & b_{m-w-1}^T \end{pmatrix}
\end{aligned}
\tag{15}
$$

where $[\widetilde{B_{m-w-1}}]$ contain unwanted Ritz values which are reduced to the real Schur form. The newly calculated diagonal component λ_{w+1} may be accepted as an eigenvalue, if $\left|\{\widetilde{b_{m+1}}\}\{\phi_{w+1}\}\right|$ satisfies the convergent condition eq.(14). Also, $\widetilde{b_{w+1}}$ can be set safely to zero, because satisfying the convergent condition guarantees the smallness of this value. If this condition is not satisfied, any other real Ritz value of $[\widetilde{B_{m-w-1}}]$ should be tested by reordering the Schur form $\begin{pmatrix} \lambda_w & * \\ & \widetilde{B_{m-w-1}} \end{pmatrix}$.

Ⅳ. RESULTS AND DISCUSSION

In this study, the total number of the elemental triangles and the nodes has been 512 and 289 respectively without differentiating TE and TM modes. The number of the edges for the implemental purpose has not been the same with each other, due to the different boundary condition applied to the surface of the waveguide. The number of TE edge is smaller than that of TM, because a few tangential components of the TE mode should be excluded at the perfectly conducting surface. The number of edges has been 736 and 800 for TE and TM modes respectively. The values of the σ used in the shift-invert strategy have been -1.0000 and 10.000 for them respectively. These values have been chosen by a few undergoing trial and error for the initial calculation of the rough inverse iteration method. The Arnoldi decomposition has been performed over the dimension $m = 20$. The tolerant value determining wanted or not wanted eigen-values for the diagonal components of the Schur matrix is chosen arbitrary



(a) 횡단전계모드 (b) 횡단자계모드
(a) TE mode (b) TM mode

그림 2. 고유치와 고유모드의 개요도
Fig. 2. Schematic representation of the eigen-values and eigen-modes.

as $Tol = 10^{-6}$. It has not been the value based on the specific theory. In the course of the calculation, several spectra have been appeared repeatedly and robustly with the Frobenius norm under this limit. So it has been set up as a pre-determined value of tolerance. The Krylov-Schur algorithm included the above mentioned processes and parameters have been carried out several times to obtain the ideally wanted eigen-pairs $c = 8$. There have been no problems to carry out the Arnoldi decomposition. The QR Algorithm has easily deduced the Schur forms from the Hessenberg matrix. There have been one or two candidates to be accepted as the wanted eigen-pairs. The unitary similar transformation has moved the eigen-pairs to the leading principle sub-matrix in the Schur form. Locking the wanted eigen-pairs and purging the unwanted Ritz-pairs could be accomplished in the deflating process very well. The Krylov-Schur decomposition could be truncated at any point without any problems. The subsequent Arnoldi process could be easily expanded from this truncated point rightly. The iteration number of that algorithm has not been exceeded five times for each TE and TM mode calculations. By doing so, all the wanted eigen-pairs $c=8$ for these modes $\{e_t\}=[\widetilde{V_w}][\Phi_w]$ have been obtained. And these modes have been plotted in the Fig.2 with the k_i^2 values resulted from converting each eigen-values into $k_i^2=\frac{1}{\lambda_i}+\sigma$.

Ⅴ. CONCLUSION

The eigen matrix equation constructed from FEM with the tangential edge vectors of the triangular elemental mesh has been calculated with the Krylov-Schur iteration method. The eigen-pairs satisfying the convergent condition have been confidentially obtained from this iteration process. The schematic representations have revealed the eigen-features of the TE and TM modes with self-consistently. From these representations, it could be certainly identified that this iteration method has been performed reliably to characterize each eigen-properties of the square waveguide. From this study, it would be expected that the eigen pairs for the varied geometrical structures such like the rectangular form etc., can be confidently obtained using the Krylov-Schur iteration method.

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