2014년 7월 전자공학회 논문지 제 51 권 제 7 호
Journal of The Institute of Electronics and Information Engineers Vol. 51, NO. 7, July 2014 http://dx.doi.org/10.5573/ieie.2014.51.7.142

논문 2014-51-7-16

Krylov-Schur 순환법을 이용한 3-차원 원통구조 도파관의 고유특성 연구

(A Study on Eigen-properties of a 3-Dim. Resonant Cavity by Krylov-Schur Iteration Method)

김 영 민*, 임 종 수**

(Yeong Min Kim© and Jong Soo Lim)

요 약

3-차원 원통 구조의 공명관에 Krylov-Schur 순환 법을 적용하였다. 균질한 매질에서 공명파의 세기를 기술하는 벡터 Helmholtz 방정식을 FEM을 이용하여 분석하였다. 고유 방정식은 사면 배위 구조 요소의 변-접선 벡터에 기반을 두어 구성하였다. 이 방정식은 Helmholtz 작용자의 curl-curl과 연관된 정방형 행렬들로 이루어져 있다. 고유-값들과 고유-모드들은 이들에 대하여 Krylov-Schur 순환 법을 적용하고, Schur 행렬의 대각 성분들과 변환 행렬들로 부터 구하였다. 결과로써 이들 고유-값과 고유-모드 쌍들을 시각적으로 묘사하였다. 그리고 각각의 경계조건에 따른 고유-쌍들을 서로 비교하였다.

Abstract

Krylov-Schur iteration method has been applied to the 3-Dim. resonant cavity of a cylindrical form. The vector Helmholtz equation has been analysed for the resonant field strength in homogeneous media by FEM. An eigen-equation has been constructed from element equations basing on tangential edges of the tetrahedra element. This equation made up of two square matrices associated with the curl-curl form of the Helmholtz operator. By performing Krylov-Schur iteration loops on them, Eigen-values and their modes have been determined from the diagonal components of the Schur matrices and its transforming matrices. Eigen-pairs as a result have been revealed visually in the schematic representations. The spectra have been compared with each other to identify the effect of boundary conditions.

Keywords : eigen-pair, Krylov-Schur, FEM, Arnoldi decomposition, QR algorithm, unitary transform.

I. INTRODUCTION

Usually the cavity resonator has the form of a volume filled with a dielectric or air. The volume is bounded by a conducting surface or by a space having differing electrical or magnetic properties. Eigen-mode analysis is a vital step during the design stage of the resonant cavity structure. Acquiring information about the eigen-pairs of the cavity gives an understanding of its resonant properties. In most cases, the resonant cavity can support an infinite number of eigen-pairs. Each eigen-pair corresponds to a unique electromagnetic field patten generated in it. This identification process can be sometimes confusing and requiring a precisely numerical

* 정회원, 경기대학교 전자물리학과경기대학교 전자물리학과
(Dept. of Elecronic Physics, Kyonggi University
© Corresponding Author(E-mail: kimym5418@hanmail.net)
접수일자: 2014년04월25일, 수정일자: 2014년06월09일
수정완료: 2014년06월24일

calculation. Especially, given the different boundary conditions make the complex eigen-pairs which can not be easily identified even in the same cavity. So. it would be resonable to study varied eigen-pairs for the cylindrical resonant cavity using the more confidential numerical algorithm.

Krylov-Schur iteration method has been known as one of the most important and actively developing algorithms for calculating the eigen-problems[1~2]. Especially, it has been recognized that this algorithm would be indispensable tool to understand the physical properties of the electromagnetic wave propagating in any cavity.

Previously, we have studied on the eigen-properties of 2-Dimensional(Dim.) waveguides of varied forms using Krylov-Schur iteration method[3~4]. The spectra of Transverse Magnetic(TM) and Transverse Electric(TE) eigen-modes and eigen-values have been revealed visually as the results. In the process of the calculation, it has been identified even more that this algorithm has been carried out robustly and drawn the eigen-pairs confidently. From these reasons, it could be recognized ones again the prominent ability of Krylov-Schur algorithm in calculating the large scale and non-symmetric eigen-problems.

To meet the demand of the periodic tendency, Krylov-Schur algorithm the same as previously studying has been applied to a 3-Dim. cavity of the cylindrical form. The eigen-equation were constructed basing on Finite Element method(FEM). The mesh element was simple tetrahedron and the shape functions were constructed with constant tangential edge vectors. In this study, it has been aim to certify the availability of Krylov-Schur algorithm for more general problems by revealing the eigen-properties of TM modes in 3-Dim. resonant cavity. As the results, the spectra for each eigen-pairs have been visualized with the schematic representations as like the previous study.

Ⅱ. FINITE ELEMENT FORMULATION

For the cavity of homogeneous media, the eigen-modes for TM and TE would be governed by the vector Helmholtz equation of dual form

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

where $k=\omega\sqrt{\epsilon_0\mu_0}$ is the 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 permittivity ϵ/ϵ_0) and, for the TM mode $\overrightarrow{F}_t=\overrightarrow{H}_t$(transverse magnetic field strength), $\nu=\epsilon_r$, $\zeta=\mu_r$. For a claim of the calculational convenience, the following description would be related to the common notation not differentiating TM or TE modes. The eigen-equations have been obtained from FEM. The Galerkin method of weighted residual has been used to construct a linear equation. In this process, boundaries of the cavity have been assumed to be PEC(perfect electric conductor). Hence, $\overrightarrow{F_t}$ for the TM and its normal derivative $\partial\overrightarrow{F_t}/\partial n$ for the TE cases may vanish at the boundary. The final equation resulted from FEM is given by

$$\iiint_V \frac{1}{\epsilon_r}(\overrightarrow{\nabla}\times\overrightarrow{T_s})\cdot(\overrightarrow{\nabla}\times\overrightarrow{F}_t)dV = k^2\mu\iiint_V \overrightarrow{T}_s\cdot\overrightarrow{F}_t dV \tag{2}$$

To avoid the spurious solution attributed to the lack of enforcement of divergence condition for $\overrightarrow{H_t}$, six basis functions have been constructed with constant tangential edge vectors $\overrightarrow{W_m}$ of the tetrahedral element[6]

$$\overrightarrow{W_m}=l_m(N_{m1}\overrightarrow{\nabla}N_{m2}-N_{m2}\overrightarrow{\nabla}N_{m1}),m=1,\ldots,6 \tag{3}$$

In this representation, N_{m1} and N_{m2} are the simplex coordinates associated with the 1st and 2nd nodes connected by the edge m, and l_m is the length of edge m. The simplex coordinates for a given elementary mesh are

$$N_n = a_n + b_n x + c_n y + d_n z, \quad n = 1, \ldots, 4 \tag{4}$$

and the gradient of any simplex coordinate is

$$\overrightarrow{\nabla} N_n = b_n \hat{x} + c_n \hat{y} + d_n \hat{z} \tag{5}$$

The simplex coefficients are calculated by inverting the coordinate matrix

$$\begin{bmatrix} a_1 & b_1 & c_1 & d_1 \\ a_2 & b_2 & c_2 & d_2 \\ a_3 & b_3 & c_3 & d_3 \\ a_4 & b_4 & c_4 & d_4 \end{bmatrix} = \begin{bmatrix} 1 & 1 & 1 & 1 \\ x_1 & x_2 & x_3 & x_4 \\ y_1 & y_2 & y_3 & y_4 \\ z_1 & z_2 & z_3 & z_4 \end{bmatrix}^{-1} \tag{6}$$

where (x_n, y_n, z_n) is a location of node n. A tetrahedron structure is given a local structure as illustrated in Fig.1. The magnetic field strength in a single tetrahedral element is represented using the tangential edge elements $\overrightarrow{W_m}$ as

$$\vec{F} = \sum_{m=1}^{m=6} e_m \overrightarrow{W_m} \tag{7}$$

The six unknown parameters associated with each edge are $e_1, \ldots, e_6$. Substituting equation (7) into equation (2), the eigen-equation for one tetrahedral element can be written in matrix form as [7]

$$[S_{el}][e] = k^2 [T_{el}][e] \tag{8}$$

where the element matrices are given by

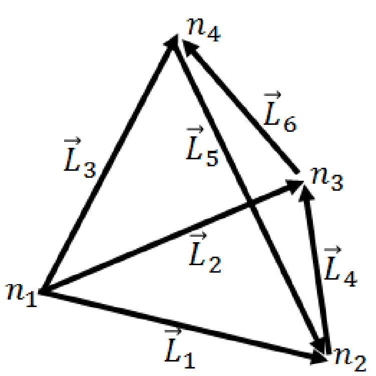


그림 1. 사면배위 단위 구조
Fig. 1. Tetrahedral structure of elemental mesh.

$$[S_{el}] = \frac{1}{\epsilon_r} \iiint_V (\overrightarrow{\nabla} \times \overrightarrow{W_m}) \cdot (\overrightarrow{\nabla} \times \overrightarrow{W_n}) dV \tag{9}$$

$$[T_{el}] = \mu_r \iiint_V (\overrightarrow{W_m} \cdot \overrightarrow{W_n}) dV \tag{10}$$

The evaluation of the element matrix $[S_{el}]$ requires the curl of each basis function $\overrightarrow{W_m}$

$$\begin{aligned} \overrightarrow{\nabla} \times \overrightarrow{W_m} &= \overrightarrow{\nabla} \times l_m (N_{m1} \nabla N_{m2} - N_{m2} \nabla N_{m1}) \\ &= 2 l_m \overrightarrow{\nabla} N_{m1} \times \overrightarrow{\nabla} N_{m2} \\ &= 2 l_m (c_{m1} d_{m2} - c_{m2} d_{m1}) \hat{x} \\ &\quad + (b_{m2} d_{m1} - b_{m1} d_{m2}) \hat{y} \\ &\quad + (b_{m1} c_{m2} - b_{m2} c_{m1}) \hat{z} \equiv 2 l_m \overrightarrow{w_m} \end{aligned} \tag{11}$$

and from it

$$[S_{el}]_{mn} = 4 l_m l_n V (\overrightarrow{w_m} \cdot \overrightarrow{w_n}) \tag{12}$$

To obtain the element matrix $[T_{el}]$, the scalar product between $\overrightarrow{W_m}$ and $\overrightarrow{W_n}$ may be calculated

$$\begin{aligned} \overrightarrow{W_m} \cdot \overrightarrow{W_n} &= l_m (N_{m1} \overrightarrow{\nabla} N_{m2} - N_{m2} \overrightarrow{\nabla} N_{m1}) \\ &\quad \cdot l_n (N_{n1} \overrightarrow{\nabla} N_{n2} - N_{n2} \overrightarrow{\nabla} N_{n1}) \\ &= l_m l_n [N_{m1} N_{n1} \psi_{m2,n2} - N_{m1} N_{n2} \psi_{m2,n1} \\ &\quad - N_{m2} N_{n1} \psi_{m1,n2} + N_{m2} N_{n2} \psi_{m1,n1}] \end{aligned} \tag{13}$$

where

$$\begin{aligned} \psi_{mi,nj} &= \overrightarrow{\nabla} N_{mi} \cdot \overrightarrow{\nabla} N_{nj} \\ &= b_{mi} b_{nj} + c_{mi} c_{nj} + d_{mi} d_{nj} \end{aligned} \tag{14}$$

In the process of $[T_{el}]$ calculation, following volume integration for 3-Dim. simplex coordinates may be used [8]

$$\iiint_V (N_1)^i (N_2)^j (N_3)^k (N_4)^l dV = \frac{3!i!j!k!l!}{(3+i+j+k+l)!} V \quad (15)$$

These integrals can be simply summarized in the matrix form as

$$[M_{ij}] = \frac{1}{V}\iiint_V N_i N_j \, dV = \frac{1}{20}\begin{bmatrix} 2 & 1 & 1 & 1 \\ 1 & 2 & 1 & 1 \\ 1 & 1 & 2 & 1 \\ 1 & 1 & 1 & 2 \end{bmatrix} \quad (16)$$

From representations (13), (14) and (16), the element matrix $[T_{el}]$ may be written as

$$[T_{el}]_{mn} = V\, l_m l_n [\psi_{m2,n2} M_{m1,n1} - \psi_{m2,n1} M_{m1,n2} - \psi_{m1,n2} M_{m2,n1} + \psi_{m1,n1} M_{m2,n2}] \quad (17)$$

These element matrices are assembled over all tetrahedral elements in the 3-Dim. cavity volume to obtain a global eigen-matrix equation.

$$[S][e] = k^2 [T][e] \quad (18)$$

Ⅲ. KRYLOV-SCHUR ITERATION METHOD

As mentioned in the previous study, it has been well known that the Krylov-Schur iteration method is the one of most reliable technique for finding the prominent eigen-pairs[9]. The method would be more

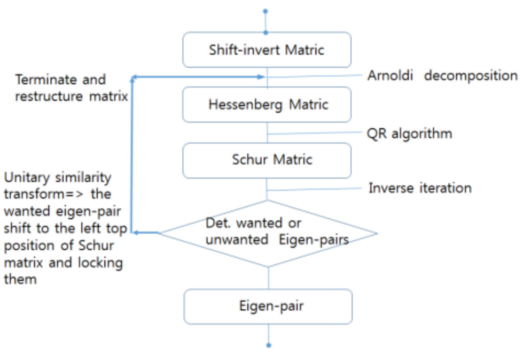


그림 2. Krylov-Schur 순환법의 계략도
Fig. 2. Block diagram for Krylov-Schur algorithm.

efficiently implemented in finding specific eigen-pairs by performing the shift-invert strategy as following

$$\frac{1}{k_c^2 - \sigma}\{e_t\} = \frac{[T]}{[S] - \sigma[T]}\{e_t\} = [M]\{e_t\} \quad (19)$$

The sparsity and symmetry of the eigen-equation would be lost, but by this strategy the convergent rate is more promoted around at the specific value σ. Subsequently, Krylov-Schur iteration method is performed on this square matrix $[M]$. It could be definitely summarized as in the Fig.2. Arnoldi decomposition compress the matrix $[M]$ into the Hessenberg matrix of dimension 20×20 by the orthogonal matrix $[Ar]$ of the dimension $n \times 20$[10]. QR algorithm with the 20×20 matrix $[Qr]$ is applied to this compressed square matrix resulting into the upper triangular Schur matrix[11]. To obtain the wanted eigen-values, inverse iteration method with $[Ir]$ is operated on this matrix[12]. The wanted eigen-values λ_w or not wanted is determined by the tolerant value Tol and the relation

$$\| [M]([V_m][\phi_w]) - \lambda([V_m][\phi_w]) \|^2 = \left|\{b_{m+1}^T\}\{\phi_w\}\right| \le \max\{u \| T_m \|_F, Tol \times \lambda_w\} \quad (20)$$

Where u and $\| * \|_F$ are the unit round off and the Frobenius norm respectively. The eigen-values would be located randomly in the diagonal position of the Schur matrix. The unitary similarity transform is carried out to shift these components to left upper position by the matrix $[Tr]$[13]. The eigen-modes corresponding to these eigen-values are resulted from the above transforming matrices by multiplying them sequently

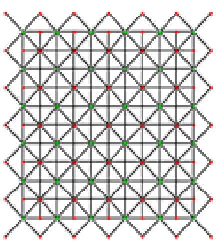
$$[e_t] = [Ar][Qr][Is][Tr] \quad (21)$$

After obtaining these eigen-pairs, they are locked and made no longer participating in the subsequent calculation for other remaindering eigen-pairs. The iterating calculations are continued subsequently restructuring the Schur matrix which is smaller than the original one by the locked components. The initial Arnoldi vector is assumed to be the last column vector of the last decomposition matrix.

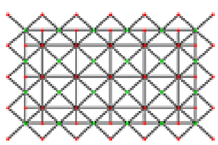
Ⅳ. TETRAHEDRAL MESH

The cavity is assumed to have a shape of cylindrical form whose magnitude of radius and height are the same with each other. The space of the cavity has been decorated with the body centered cubic lattice as a first step of mesh constructing process. The mesh elements of the tetrahedral structure have been made by connecting the four lattice points as exhibited in Fig. 3. Fig. 3 (a) and (b) is the feature of the initial mesh projected in the xy and yz plane respectively. The tetrahedral elements laying outside the boundaries must be reconstructed because of including the non-meaningful space outside the cavity. The space running over the boundaries could be excluded from the boundaries.

The nodes positioned over the surface could be shifted to the boundaries. The edge lengths of element meshes deformed by them may be remedied to recover the shape of tetrahedral structure. The resulting mesh has been represented on the cavity as can be seen in Fig. 4. The eigen-equation has been constructed from FEM based on this tetrahedral mesh. The eigen-pairs have been calculated by applying Krylov-Schur iteration method to this equation.



(a)



(b)

그림 3. (a) xy-면 및 (b) yz-면에 투영된 단위 요소
Fig. 3. Mesh projected on.
(a) xy-plane and (b) yz-plane.

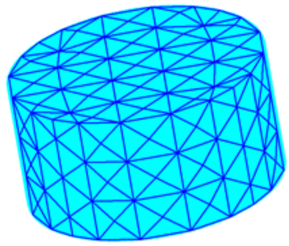


그림 4. 3-차원 요소
Fig. 4. 3-Dim. mesh.

Ⅴ. RESULTS AND DISCUSSION

In this study, the eigen-pairs for the cylindrical resonant cavities with different boundary conditions were compared with each other. The one has been assumed that the lateral boundary surface coated with the perfectly conducting metal, and the other did not given any restriction. In the process of calculational implementation, the former condition was accommodated by ignoring the variables for the tangential edge vectors on the surface. The space occupied by the cavity was assumed to be linear and homogeneous. So, it not been worried any leakage and anisotropic field variation in the calculation.

It was assumed that the cylindrical resonant cavity has the finite length along the direction of propagating wave. It was also assumed that the radius and height of them are given with the same sizes arbitrary. The structure The mesh in this study were constructed by tetrahedral unit structures for the space of the cavity excluding the surfaces. Around these places, systematic remedying for the tetrahedra has been made by shifting the node points and adjusting the edge lengths. For the three dimensional problem, the number of variables increases drastically compared with those for two dimensional problems. The numbers of node, mesh and edge in this study have been 389, 992 and 1780 respectively resulting by remedying and refining the raw mesh. Krylov-Schur iteration method have been carried out as mentioned in the Fig. 2. which is the same as the previous studies[3~4]. The iterative loops have been performed satisfactory to ensure its robustness. The most important and time consumptive process in this iteration loop is the calculation of the inverse matrix for the square matrix $[M]$. The edge number has not caused any trouble in calculating the inverse matrix by LU decomposition method even using personal computer.

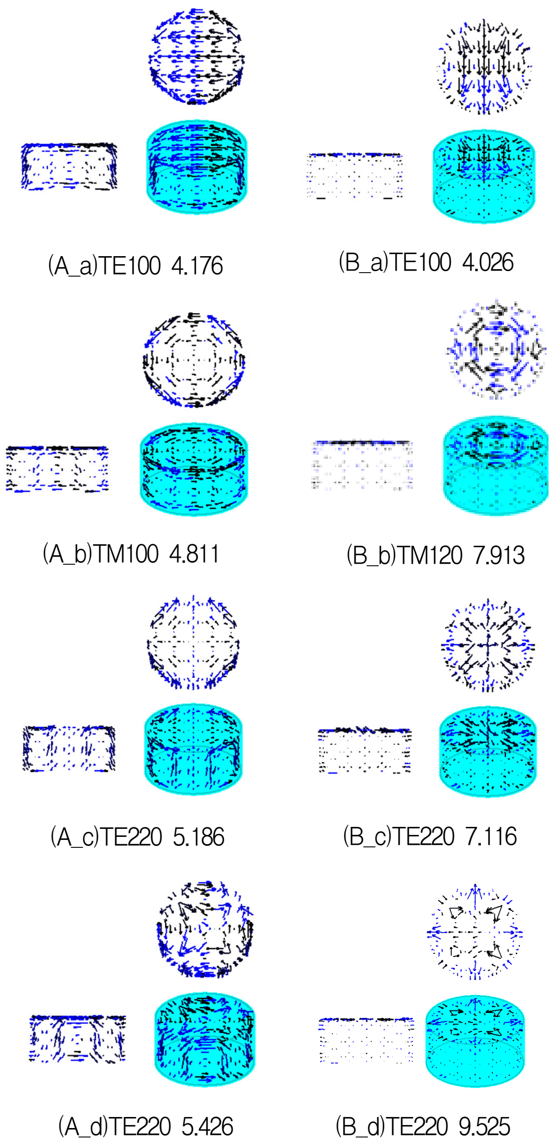


그림 5. 원통형 공명관의 고유모드와 파수(cm^{-1})
Fig. 5. Eigen-modes and eigen-values(cm^{-1}) of the cylindrical resonant cavities.

In determining the eigen-pairs, a tolerant value have been a value about $Tol \sim 10^{-3}$ which is larger than that of 2-Dim. cases. The eigen-values have been calculated by converting each diagonal components of the Schur matrix into values $k_i^2 = \dfrac{1}{\lambda_i} + \sigma$ reversing the shift-invert strategy. Wave numbers have been calculated by taking square root values on them. The resulting eigen-pairs have been revealed schematically in the Fig.5. The spectra were arranged with characteristic wave numbers about the values 2-10cm^{-1}. In figures, spectra named by A_series are for the cavity without any restriction. Spectra represented by B_series are for the cavity whose lateral surface have been coated with the perfectly conducting metal. 3-Dim. spectra have been accompanied with the 2-Dim. spectra which are resulted by projecting them on the xy and yz plains. The mode-types were determined by comparing them with those of the reference[14]. As can be seen from this figure, it may be identified that spectra A_series and B_series have been sufficiently reflected the properties of each boundary conditions. The spectra (A_a) and (B_a) have revealed the similar properties of TE100 modes. The difference appeared at the circumference around the lateral surfaces. As increasing the wave numbers, the similarity was disappeared. The spectra were seemed to show their intrinsic properties depending on their boundary conditions. The spectra have been shown no variation in z-direction. It would be come from the difference of height relatively small compared to the radius.

Ⅵ. Conclusion

The Krylov-Schur iteration method has been applied to the 3-Dim. resonant cavities of the cylindrical form. Cavities have different lateral boundary conditions. The eigen-pairs satisfying the convergent condition have been obtained. It has seemed that the boundary conditions were sufficiently reflected on the spectra. From these results, it has been certified that the spectra have revealed the characteristics of the eigen- properties of the cavity under different boundary conditions. Together with the results from calculations of 2-Dim. waveguides, it was successfully confirmed that Krylov-Schur algorithm could be applied to varied physical structures.

REREFENCES

[1] G. W. Stewart, "A Kryliv Schur Algorithm for Large Eigenproblems" SIAM J. Matrix Anal. & Appl. 23(3), 601 (2002).
[2] G. W. Stewart, "Addendum to 'A Krylov-Schur Algorism for Large Eigenproblems" SIAM J. Matrix Anal. & Appl. 24(2), 599 (2002).
[3] Yeong Min Kim, Dongchool Kim and Jong Soo Lim, "A Study on The Eigen- properties of A 2-D Square Waveguide by the Krylov-Schur iteration method" Journal of The Institute of Electronics Engineers of Korea Vol. 50. NO. 11, November 2013.
[4] Yeong Min Kim, Dongchool Kim and Jong Soo Lim, "A Study on The eigen- properties on Vaired structural 2-Dim. Waveguides by Krylov-Schure Iteration Method" Journal of The Institute of Electronics Engineers of Korea Vol. 51. NO. 2, Faburary 2014.
[5] C. J. Reddy, Manohar D. Deshpande, C. R. Cockrell, and Fred B. Beck, "Finite Element Method for Eigenvalue Problems in Electromagnetics" NASA Technical Paper 3485(1994).
[6] Alexandre Nentchev, "Numerical Analysis and Simulation in Microelectronics by Vector Finite Elements" Ph. D. thesis, Vienna University of technology, 2008.
[7] J. Scott Savage, and Andrew F. Peterson, "Higher-Order Vector Finite Elements for Tetrahedral Cells" IEEE Trans. Microwave theory Tech. Vol. 44, No. 6, June 1996.
[8] P. Silvester and R. Ferrari, *Finite Elements for Electrical Engineering*, 3th ed.(Cambridge University Press, New York,1996), p. 183.
[9] V. Hernández, J. E. Román, A. Tomás and V. Vidal,"Krylov-Schur Methods in SLEPc" SLEPc Technical Report STR-7 (2007).
[10] V. Hernández, J. E. Román, A. Tomás and V. Vidal, "Arnoldi Methods in Sleps" SLEPc Technical Report STR-4.(2006).
[11] David S. Watkins, "The QR Algorithm revisited" SIAM Rev. 50, 133 (2008).
[12] Maysum Panju, "Iterative Methods for Computing Eigenvalues and Eigenvector" The Waterloo Math. Rev.1, 9(2011).
[13] Z. Bai, J. W. Demmel, "On Swapping Diagonal Blocks in Real Schur Form" Linear Algebra Appl. 186, 73 (1993).
[14] J. P. KINZER and I, G. WILSON. "End Plate and Side Wall Currents in Circular Cylinder Cavity Resonator" http://www3.alcatel-lucent.com/bstj/vol26-1947/articles/bstj26-1-31.pdf

저 자 소 개

김 영 민(정회원)
1985년 경기대학교 물리학 학사
1997년 동국대학교 물리학 석사
1996년 동국대학교 물리학 박사
2012년~2014년 현재 경기대학교 전자물리학과 초빙교수

<주관심분야 : 고체물리학, 전산물리>

임 종 수(정회원)
1970년 성균관대학교 천체 지구물리학 석사
1980년 성균관대학교 응용물리학 석사
1984년 성균관대학교 응용물리학 박사
1981~2012년 경기대학교 물리학과 교수
1993~1995년 죠지워싱턴대학교 교환교수
1995~1997년 경기대학교 자연과학대학 학장
1997~1999년 경기대학교 종합평가위원장
2013~2014년 현재 경기대학교 명예교수
<주관심분야 : 응용물리, 초음파 및 후학 육성>