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AN EFFICIENT APPROACH FOR MULTIFRONTAL ALGORITHM TO SOLVE NON-POSITIVE-DEFINITE FINITE ELEMENT EQUATIONS IN ELECTROMAGNETIC PROBLEMS

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Abstract—A new method called Expanded Cholesky Method (ECM) is proposed in this paper. The method can be used to decompose sparse symmetric non-positive-definite finite element (FEM) matrices. There are some advantages of the ECM, such as low storage, simplicity and easy parallelization. Based on the method, multifrontal (MF) algorithm is applied in non-positive-definite FEM computation. Numerical results show that the hybrid ECM/MF algorithm is stable and effective. In comparison with Generalized Minimal Residual Method (GMRES) in FEM electromagnetic computation, hybrid ECM/MF technology has distinct advantages in precision. The proposed method can be used to calculate a class of non-positive-definite electromagnetic problems.

1. INTRODUCTION

There are many numerical methods, such as the finite element method (FEM) [1–4], finite-difference time-domain (FDTD) [5–9], and moment of methods (MOM) [10], have been applied to analyze electromagnetic problems. For the analysis of complex structures, the FEM is applied to electromagnetic problems in this paper. It is a key of FEM to solve the equations like $AX = B$, which are sparse symmetric linear. The iterative algorithms [11, 12] and direct methods [13, 14] are employed to carry out the equations usually. The convergence rate of iterative methods is mainly determined by the condition number of coefficient matrix. However, due to the complexity of targets' material and shape, the FEM matrix is ill-conditioned which leads to a very slow convergence rate or even nonconvergence of the iterative solutions.

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As iterative methods are invalid in some cases, direct methods are employed in this paper. One of the significant advancements in direct methods for a sparse matrix solution is the development of the multifrontal (MF) algorithm [15–18]. The algorithm is an effective method for solving large-scale sparse linear equations. There are some advantages of this approach over other factorization algorithms, such as better data locality, effective vector processing on dense frontal matrices, etc. [19].

MF algorithm is based on LU decomposition method, and it is carried out in accordance with the order of elimination tree. LU decomposition method is usually replaced by Cholesky decomposition method in symmetric problems. Cholesky decomposition method only operates half of the matrix. For the triangular decomposition, the Cholesky decomposition method can save half of calculation of LU decomposition method [20]. The Cholesky decomposition method is simple and easy to perform parallel process. Cholesky decomposition method is one of the most numerically stable algorithms [21]. Therefore, this method is employed in the MF technology.

As Cholesky decomposition method is based on the assumption of a positive-definite pattern, the MF algorithm is a kind of solution scheme for positive-definite systems. However, in many electromagnetic (EM) problems, such as calculating the scattering from a dielectric cube on the PEC plate, where the diagonal entries of the coefficient matrix A may be complex. Obviously, it means that $AX = B$ are non-positive-definite finite element equations; Cholesky decomposition method will be invalid. For the case that will generate a sparse symmetric complex (not real) matrix whose sequential principal minor determinants are not equal to zero, and it can be expressed as

$$A_k = \begin{vmatrix} a_{11} & a_{12} & ,\ldots, & a_{1n} \\ a_{21} & \ddots & & \vdots \\ \vdots & & \ddots & \vdots \\ a_{n1} & ,\ldots, & ,\ldots, & a_{nn} \end{vmatrix} \neq 0 \qquad (k = 1, 2, n) \ .$$

In order to decompose the matrices, a new method called Expanded Cholesky Method (ECM) is proposed in this paper.

The ECM provides an exact solution of symmetric non-positive-definite problems which can not be solved by Cholesky decomposition method, and it is introduced to the MF algorithm for the FEM method. The comparison with GMRES method shows that the MF algorithm using ECM is correct and stable. Based on this method, the FEM algorithm is applied successfully to solve the complex electromagnetic problems. Numerical results demonstrate that the proposed algorithm can be used to calculate a class of non-positive-definite electromagnetic problems.

This paper is organized as follows. Section 2 presents the basic and optimized procedure of MF algorithm. In Section 3, the ECM and its demonstration are presented, and the application of ECM in MF algorithm is described. In Section 4, some FEM results obtained by the hybrid ECM/MF approach are presented and compared with GMRES method. Finally, conclusions are outlined in Section 5.

2. BASIC THEOREM

According to the analysis of finite element method [1], the calculation of scattering problems focus on the solution of the equations

$$AX = B, \tag{1}$$

where A is a sparse linear matrix and B is a column vector, both of them are not equal to zero.

Following by the LU decomposition, the coefficient matrix A in (1) is decomposed as product of two triangular matrices

$$A = LU, \tag{2}$$

where L and U are lower and upper triangular matrices respectively. Then (2) can be rewritten as

$$LUX = B. \tag{3}$$

Y is defined by

$$Y = UX, \tag{4}$$

and (3) can be further rewritten as

$$LY = B. \tag{5}$$

Then Y can be solved through forward elimination,

$$y_i = b_i - \sum_{k=1}^{i-1} l_{ik} y_k \quad (i = 1, 2, \ldots, n) \tag{6}$$

and backward substitution is used to seek the ultimate solution X

$$x_i = \left(y_i - \sum_{k=i+1}^{n} u_{ik} x_k \right) \Big/ u_{kk} \quad (i = n, n-1, \ldots, 1)\,. \tag{7}$$

In the MF computation process, the sparse matrix is firstly re-organized into a series of dense one, which is called fill-ins reducing method. Then, dense matrices are carried out in low-level decomposition, by which the matrices only with the low-level-related border unknowns of wavefront matrix are obtained. Finally, all the adjacent public unknowns between the low-level matrices are eliminated, and the process is given by formula (3)–(7).

The fill-ins reducing work is a key of the MF algorithm. In order to minimize fill-ins number, some fill-ins reducing algorithms [21–23] are developed. The approximate minimum degree ordering algorithm [23] is chosen here as a fill-reducing method.

Besides the approximate minimum degree ordering algorithm, a further optimization is needed. The optimization algorithm is explained bellow. In accordance with the conclusions of the literature [24], the fill-ins of the matrix A are identified firstly: If $j = parent(k)$, and $l_{ik} \neq 0$, then it certainly has $l_{ij} \neq 0$, where j is the first row number of non-zero element following the diagonal element in column k, and $parent(k)$ is the father node of k. Then the corresponding elimination tree can be constructed. After that, the tree is updated in postorder to generate a new sequence of nodes. According to the generated sequence, the fill-ins and the elimination tree can be re-identified by the same way. In order to minimize the storage consuming, the subtree of the node j needs to be reordered in a descending order [24], which can be expressed as

$$\max\left\{ms(c_i), |F_j|\right\} - |U_{c_i}|, \tag{8}$$

where c_i is the son of node j in the elimination tree; $|F_j|$ is the number of non-zero elements of frontal matrix F_j; $|U_{c_i}|$ is the number of non-zero elements of update matrix U_{c_i}; $ms(c_i)$ is the minimum working space. Subsequently, let $r = size(col(j))$, where r denotes the number of non-zero elements of the column j; formulas can be obtained as follows:

$$|F_j| = \frac{1}{2}r\,(r+1)\,,\ \ |U_j| = \frac{1}{2}r\,(r-1)\,, \tag{9}$$

$$ms(j) = \max_{1\leq k\leq s}\left\{\max\left\{ms(c_k), |F_j|\right\} + \sum_{i=1}^{k-1}|U_{c_i}|\right\}. \tag{10}$$

In order to facilitate the description, the optimized equations are still referred to as $AX = B$. The MF improves the calculating efficiency by changing the order of the factorization.

As described in introduction, the complex linear finite element equations obtained from most of the electromagnetic problems are sparse symmetric that are not positive definite. Generally, LU decomposition or the MF based on LU decomposition can be used to deal with this kind of problems, but all of the direct methods available except Cholesky decomposition method need to store and compute non-zero elements and fill-ins of whole matrix, which is very time and space consuming. As only half of matrix needs to be stored and calculated, the MF algorithm based on Cholesky decomposition method is usually used, but only the positive-definite matrix can be decomposed with this method. An Expanded Cholesky Method is proposed here to decompose the non-positive-definite matrix in high efficiency and accuracy.

3. EXPANDED CHOLESKY METHOD

The Cholesky decomposition method deals with only half of the coefficient matrix, and the amount of calculation is reduced by nearly half. However, the method has a strong constraint, namely positive definiteness. For most of the electromagnetic analysis, the coefficients matrices of FEM are complex and not Hermitian. As the algorithm is invalid for the matrices are complex but not positive definite, the ECM method is proposed here.

According to the constraint of the Cholesky algorithm, if A in (1) has complex entries and is positive-definite Hermitian matrix, then there exists a unique lower triangular matrix L with strictly positive diagonal elements, that allows the factorization of A into $A = LL^*$, where L^* is the conjugate transpose of L. The entries on the main diagonal of any Hermitian matrix have to be real. If A is complex symmetric and not positive definite, the original Cholesky algorithm does not work. In the case of complex symmetrical matrix whose sequential principal minor determinants are not equal to zero, a method called ECM is developed here. The ECM decomposes A as

$$A = LL^T, \tag{11}$$

where L^T denotes the transpose of L. The following formula is for the entries of L,

$$\begin{cases} L_{i,j} = \frac{1}{L_{j,j}}\left(A_{i,j} - \sum\limits_{k=1}^{j-1} L_{i,k}L_{j,k}\right), \\ L_{i,i} = \sqrt{A_{i,i} - \sum\limits_{k=1}^{j-1} L_{i,k}^2}, \end{cases}$$

when $i > j$.

The following is the proof of the proposed decomposition approach.

According to the uniqueness of $\tilde{L}\tilde{D}U$ decomposition, A has a unique triangular decomposition when the sequential principal minor determinants of A are not equal to zero,

$$A = \tilde{L}\tilde{D}U \tag{12}$$

where $\tilde{L}$ is a unit lower triangular matrix; U is a unit upper triangular matrix; $\tilde{D} = \text{diag}(d_1, d_2, \ldots, d_n)$. The root of $\tilde{D}$ is computed in the complex field, that is, $D = \text{diag}(csqrt(d_1), csqrt(d_2), \ldots, csqrt(d_n))$. Thus, the new decomposition form of A can be given by

$$A = \tilde{L}\,(D)^2\,U. \tag{13}$$

A is symmetry, so

$$A^T = A. \tag{14}$$

Then (15) is obtained when (14) is substituted with (13).

$$U^T\,(D)^2\,\tilde{L}^T = \tilde{L}\,(D)^2\,U \tag{15}$$

By the uniqueness of the $\tilde{L}\tilde{D}U$ decomposition, we can get (16) as follows:

$$\tilde{L} = U^T,\ \ \tilde{L}^T = U. \tag{16}$$

With these substitutions, (12) takes the form shown in (17)

$$A = \tilde{L}\,(D)^2\,\tilde{L}^T = LL^T \tag{17}$$

where $L = \tilde{L}D$.

Only half of the matrix A needs to be stored and computed in the proposed algorithm. For complex symmetric non-positive-definite equations, the coefficient matrix A can be decomposed as (17).

The decomposition process of submatrix-ECM can be expressed as

$$\begin{aligned} A &= \begin{bmatrix} d & V^T \\ V & C \end{bmatrix} = \begin{bmatrix} \sqrt{d} & 0 \\ V\big/\sqrt{d} & I \end{bmatrix} \begin{bmatrix} I & 0 \\ 0 & C - VV^T/d \end{bmatrix} \begin{bmatrix} \sqrt{d} & V^T\big/\sqrt{d} \\ 0 & I \end{bmatrix} \\ &= \begin{bmatrix} \sqrt{d} & 0 \\ V\big/\sqrt{d} & I \end{bmatrix} \begin{bmatrix} I & 0 \\ 0 & H \end{bmatrix} \begin{bmatrix} \sqrt{d} & V^T\big/\sqrt{d} \\ 0 & I \end{bmatrix} \\ &= \begin{bmatrix} \sqrt{d} & 0 \\ V\big/\sqrt{d} & I \end{bmatrix} \begin{bmatrix} I & 0 \\ 0 & L_H \end{bmatrix} \begin{bmatrix} I & 0 \\ 0 & L_H^T \end{bmatrix} \begin{bmatrix} \sqrt{d} & V^T\big/\sqrt{d} \\ 0 & I \end{bmatrix} \\ &= \begin{bmatrix} \sqrt{d} & 0 \\ V\big/\sqrt{d} & L_H \end{bmatrix} \begin{bmatrix} \sqrt{d} & V^T\big/\sqrt{d} \\ 0 & L_H^T \end{bmatrix} \\ &= LL^T \end{aligned} \tag{18}$$

where d is the first diagonal element of the matrix; V^T is the transpose of V; C is a $(n-1)\times(n-1)$-order matrix which is derived after removing the first row and column from the matrix A; C-VV^T/d expresses the subtree which will be decomposed by the similar process [18]. To the

kth decomposition, the contribution U_k of the sub-tree of node k to its ancestors can be expressed as

$$U_k = -\sum_{p\in T[k]} \begin{pmatrix} l_{i_1,p} \\ l_{i_2,p} \\ \vdots \\ l_{i_r,p} \end{pmatrix} \begin{pmatrix} l^T_{i_1,p} & l^T_{i_2,p} & ,\ldots, & l^T_{i_r,p} \end{pmatrix}. \tag{19}$$

Let the children of node k in the elimination tree be $c_1, c_2, \ldots, c_r$, the relationship between frontal matrix $\{F_k\}$ and update matrix $\{U_k\}$ can be expressed as

$$F_k = \begin{bmatrix} a_{k,k} & a^T_{i_1,k} & ,\ldots, & a^T_{i_r,k} \\ a_{i_1,k} & & & \\ \vdots & & 0 & \\ a_{i_r,k} & & & \end{bmatrix} + U_{c_1} + U_{c_2} +, \ldots, +U_{c_r}. \tag{20}$$

The decomposition is repeated until the corresponding decomposition and updating are completed. In the decomposition process, only the first column of the F_k needs to be stored.

4. NUMERICAL RESULTS

The validity and the effectiveness of the MF algorithm based on the ECM will be illustrated by numerical examples in this section.

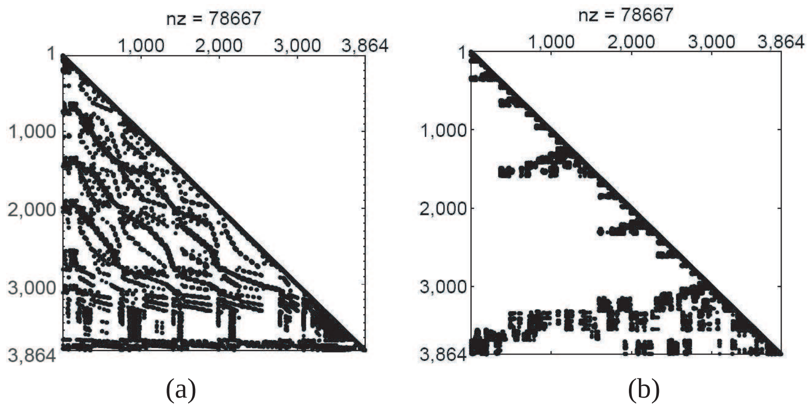

Figure 1. Distribution of 3864-order coecient matrix. (a) Lower triangular coecient matrix before optimizing after optimizing. (b) Lower triangular coecient matrix.

4.1. 3864-order Equations

There are 153,407 non-zero elements in the 3864-order matrix. The coefficient lower triangular matrix distributions of non-zero elements are given in Fig. 1. From Fig. 1, it can be seen more clearly that the distribution of non-zero elements in the optimized matrix is more regular and zoster than that of non-zero elements in the original matrix. The extra storage space occupied by non-zero elements in the follow-up calculation is significantly reduced. Let $error(i) = A^* x(i) - b(i)$, $i = 1, 2, \dots, 3864$. Respectively, the real and imaginary parts of errors are given as shown in Fig. 2, where A is the 3864-order coefficient matrix. The errors are all -5 orders of magnitude. The proposed method is considerable stable and accurate.

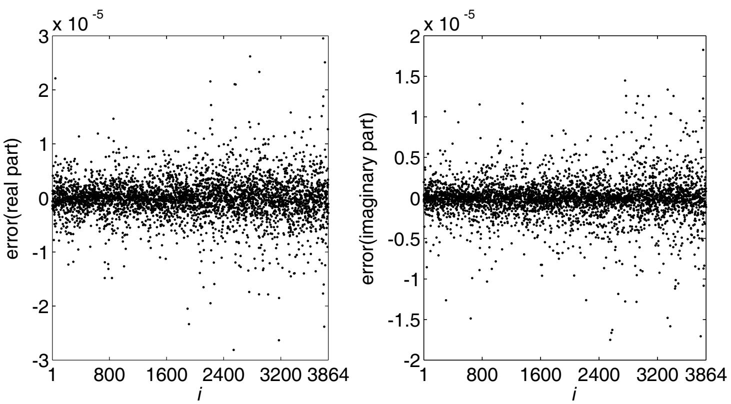

Figure 2. Errors computed by the MF algorithm using the ECM.

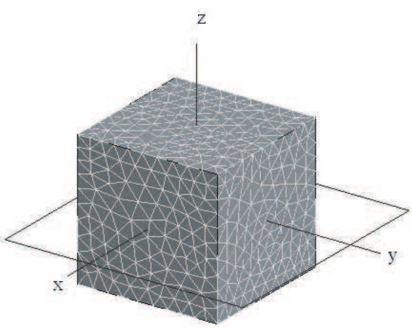

Figure 3. A cube with the side length is $0.755\lambda_0$.

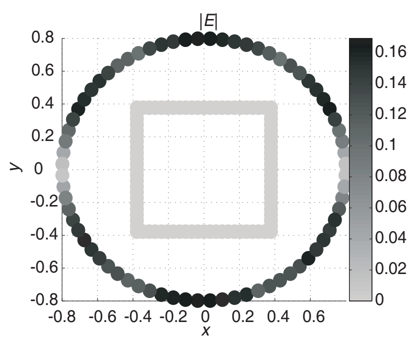

Figure 4. Field distribution at $z = 0$ cross-section.

4.2. Scattering of a PEC Cube

The second example is a PEC cube having a side length of $0.755\lambda_0$, where λ_0 is the wavelength in free space. By the proposed method, the scattering cross-section field distribution map of the PEC cube is shown in Fig. 3. Assuming a plane wave is exited, the incident wave travels in the negative z direction, and the direction of polarization is x direction. The finite element linear equations can be described as follows: Its coefficient matrix has 16,307 unknowns, and the number of non-zero elements is 234,605.

Figure 4 shows the field distribution at $z = 0$ cross-section. With field amplitude increases, gray-scale deepens. Let $error(i) = A^*x(i) - b(i)$, $i = 1, 2, \ldots, 16, 307$. A comparison of the results obtained by the ECM and GRMES is shown in Fig. 5. Generally, GMRES convergence setting uses the relative error norm $\delta_0 = 0.001$. Comparative results show that the proposed method is more accurate.

4.3. Scattering of a Dielectric Cube on the PEC Plate

Finally, a dielectric cube on the PEC plate as shown in Fig. 6 is computed. The parameters of the scatterer are given as follows: The relative permittivity of the computational domain $\varepsilon_r = 2.25$; the size of the dielectric thick layer is $0.4\lambda_0 * 0.4\lambda_0 * 0.2\lambda_0$; the size of PEC bottom board is $0.4\lambda_0 * 0.4\lambda_0$, where λ_0 is the wavelength in free-space. Also assuming a plane wave is exited, the incident wave travels in the negative z direction, and the direction of polarization is X direction. The 3D problem has 39,688 unknowns, and the number of non-zero elements is 626,146.

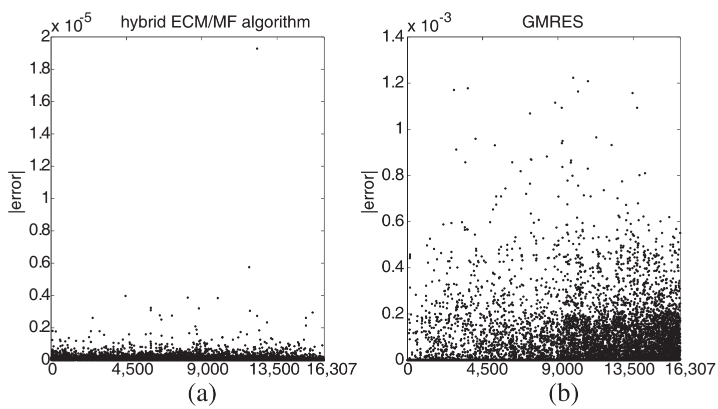

Figure 5. Errors computed by the hybrid ECM/MF algorithm and GMRES, respectively.

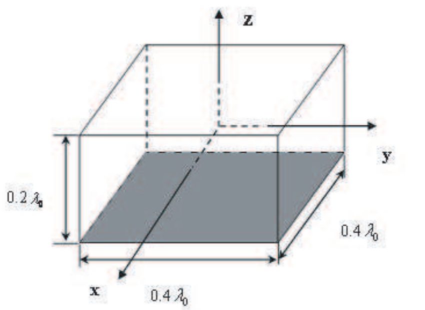

Figure 6. A dielectric cube on the PEC plate.

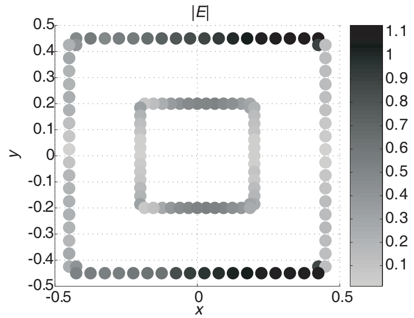

Figure 7. Field distribution at $z = 0$ cross-section.

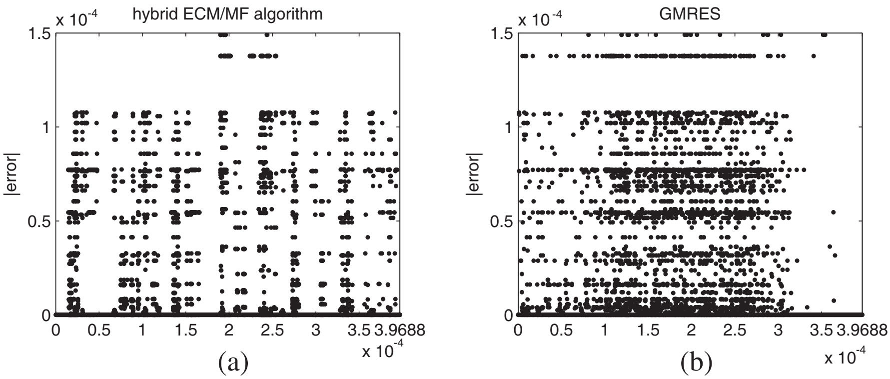

Figure 8. Errors computed by the hybrid ECM/MF algorithm and GMRES, respectively.

Due to computer error, the matrix from the finite element calculation emerges 264 points (points of upper and lower triangular matrix is 528) which have symmetric position and non-symmetric values. Because $|a_{ij} - a_{ji}|$ are all in the range of -20 the order of magnitude, the matrix can be approximated as a symmetric matrix. The field amplitude distribution calculated by the proposed method is shown in Fig. 7. As field amplitude increases, gray-scale deepens in figure.

Let $error(i) = A^*x(i) - b(i)$, $i = 1, 2, \ldots, 39,688$. A comparison of the results obtained by the ECM and GRMES is shown in Fig. 8. The computation results show that the MF algorithm based on the ECM is valid in complex non-positive definite electromagnetic problems.

5. CONCLUSION

In this paper, an efficient approach for electromagnetic computation of sparse symmetric non-positive-definite linear equations has been proposed. This approach uses a proposed new decomposition method called ECM and solves the FEM equations with MF technique. Optimization methods for reducing the extra demand of fill-ins storage space have been discussed. A number of non-positive-definite examples of electromagnetic computation illustrate the successful application of the hybrid ECM/MF approach, and the results show that the technique proposed is better than GMRES. An apparent advantage of the ECM is accuracy and potential hybridization with some iterative methods. Future study on the ECM is to make greater use of non-positive-definite hybridization techniques to increase the method's efficiency while retaining its inherent low storage, simplicity and easy parallelization.

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