Complex Incomplete Cholesky Factorization Preconditioned Bi-conjugate Gradient Method

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***Abstract*—** Linear systems generated by finite element method (FEM) always have a symmetrical sparse system matrix, which requires a large amount of computation and memory effort to access its zero elements. To address this problem, a fully-sparse storing scheme is proposed to store only nonzero symmetrical elements of the sparse system matrix. Meanwhile, for some ill-conditioned system matrixes, conventional iterative solution methods may incur such problems as slow convergence and even failure of convergence. To solve this problem, we further develop a fast convergent preconditioned bi-conjugate gradient method (PBCG) based on a real incomplete Cholesky factorization preconditioner. Numerical experiments show that the proposed method accelerates the convergence and is applicable for the large-scale complex linear systems.

***Index Terms*—** Bi-conjugate gradient method, complex sparse linear system, incomplete Cholesky factorization preconditioner.

SYMBOLS

$C^{n\times n}$	$n\times n$ complex matrix
C^{n}	n complex vector
$R^{n\times n}$	$n\times n$ real matrix
R^{n}	n real vector
$\boldsymbol{A}^{*}$	conjugate matrix
$\boldsymbol{A}^{-1}$	inverse matrix
$\boldsymbol{x}^{*}$	conjugate vector
α^{*}	conjugate complex number
ε	error
$\|\cdot\|$	Euclidean norm
$(\cdot,\cdot)$	Euclidean product
iters	number of iterations
time	time of iterations, unit is second

I. INTRODUCTION

Many electromagnetic numerical evaluations are involved in solving large-scale complex linear systems. Direct methods generally require heavy storage and computation load. As alternative approaches, high-performance iterative methods have been attracting more and more attentions in solving the complex linear system in recent years. However, if the complex linear system is of very high dimension or its system matrix is ill-conditioned, iterative methods may incur such problems as slow convergence and even failure of convergence. Fortunately, these problems can be addressed by appropriate preconditioning methods [1-3]. One most frequently used preconditioned method is the incomplete Cholesky factorization algorithm. In this paper, a real incomplete Cholesky factorization algorithm is extended into the complex field, and a complex incomplete preconditioned bi-conjugate gradient method is proposed to solve the complex large scale linear systems.

The efficiency of solving large-scale sparse complex linear systems, also, depends on storing methods for system matrixes. In order to save storage space and access the elements conveniently, we introduce a fully-sparse storing scheme that stores only nonzero symmetrical elements of system matrix by a chain pattern. Compared with current popular storing methods, the proposed method has the least storing scale and is obviously advantageous for large-scale sparse matrixes especially.

The contents of this paper include the fully-sparse storing scheme, complex incomplete preconditioned bi-conjugate gradient method,

algorithmic implementation, and numerical experiments, which demonstrate both applicability and effectiveness of the proposed method.

II. FULLY-SPARSE STORING SCHEME

An efficient fully-sparse storing scheme is presented for storing the system matrix by exploiting its properties of sparsity and symmetry. In this fully-sparse database, only nonzero symmetrical elements of system matrix are stored by using a chain pattern. Both single chain and double chain are applicable in the dynamic database. In this section, the sparse storage scheme based on a single chain pattern is presented. Extension to double chain is straightforward.

For a symmetric sparse matrix $\boldsymbol{A} \in \mathrm{C}^{n\times n}$, four one-dimension arrays are necessary to store and manage its nonzero elements. These arrays are defined as follows:

(1) Real array named DATA stores nonzero elements of lower triangle part of matrix $\boldsymbol{A}$, row by row.

(2) Integer array named JCOL stores column numbers of the nonzero elements in the array DATA.

(3) Integer array named LINK stores index numbers of the nonzero elements. For instance, in some row the index number of the *i*th nonzero element is the address of next nonzero element in the array DATA. If the *i*th nonzero element is the last element stored in this row, then LINK(*i*)=0.

(4) Integer array named HEAD stores address of first nonzero element of every row in the array DATA.

For example, if a symmetric sparse matrix $\boldsymbol{A} \in \mathrm{C}^{5\times 5}$ is expressed in equation (1), the four storing arrays in the full-sparse database are shown in Table 1.

$$\boldsymbol{A} = \begin{bmatrix} a_{11} & a_{12} & 0 & a_{14} & 0 \\ a_{21} & a_{22} & 0 & 0 & a_{25} \\ 0 & 0 & a_{33} & 0 & 0 \\ a_{41} & 0 & 0 & a_{44} & 0 \\ 0 & a_{52} & 0 & 0 & a_{55} \end{bmatrix} \tag{1}$$

Table 1: Full-sparse storing arrays

NE	1	2	3	4	5	6	7	8
DATA	a_{11}	a_{21}	a_{22}	a_{33}	a_{41}	a_{44}	a_{52}	a_{55}
JCOL	1	1	2	3	1	4	2	5
LINK	0	3	0	0	6	0	8	0
HEAD	1	2	4	5	7			

In this full-sparse database, all nonzero elements can be accessed conveniently. Basic dynamic operations are realized easily by simple searching, inserting, and deleting arithmetic. It is worth mentioning that the advantage of the proposed fully-sparse storing database is even significant for large-scale sparse matrix.

III. BI-CONJUGATE GRADIENT METHOD

Conventional iterative methods such as the conjugate gradient (CG) method [4] and the preconditioned conjugate gradient (PCG) method [5, 6] are based on real linear systems. When it comes to complex linear systems, new iterative methods are still open to be developed. In this section, a new method for solving symmetrical complex linear systems is proposed by regaining the basic concept of the bi-conjugate gradient method (BCG) for solving nonsymmetrical complex linear systems.

For symmetrical complex linear systems $\boldsymbol{Ax} = \boldsymbol{b}$, the modified BCG consists of the following steps:

Step 1: Set $i = 0$, input matrix $\boldsymbol{A} \in \mathrm{C}^{n\times n}$, vector $\boldsymbol{b} \in \mathrm{C}^{n}$, initial vector $\boldsymbol{x}_i \in \mathrm{C}^{n}$ and error criterion ε, compute $\boldsymbol{r}_i = \boldsymbol{b} - \boldsymbol{A}\boldsymbol{x}_i$, $\hat{\boldsymbol{r}}_i = \boldsymbol{r}_i^*$, $\boldsymbol{p}_i = \boldsymbol{r}_i$, and $\hat{\boldsymbol{p}}_i = \hat{\boldsymbol{r}}_i$;

Step 2: Increase index i by 1 and calculate:

$\alpha_i = (\hat{\boldsymbol{r}}_i, \boldsymbol{r}_i)/(\hat{\boldsymbol{p}}_i, \boldsymbol{A}\boldsymbol{p}_i)$, $\boldsymbol{x}_{i+1} = \boldsymbol{x}_i + \alpha_i \boldsymbol{p}_i$,

$\boldsymbol{r}_{i+1} = \boldsymbol{r}_i - \alpha_i \boldsymbol{A}\boldsymbol{p}_i$, $\hat{\boldsymbol{r}}_{i+1} = \hat{\boldsymbol{r}}_i - \alpha_i^* \boldsymbol{A}^* \hat{\boldsymbol{p}}_i$;

$\beta_i = (\hat{\boldsymbol{r}}_{i+1}, \boldsymbol{r}_{i+1})/(\hat{\boldsymbol{r}}_i, \boldsymbol{r}_i)$, $\boldsymbol{p}_{i+1} = \boldsymbol{r}_{i+1} + \beta_i \boldsymbol{p}_i$,

$\hat{\boldsymbol{p}}_{i+1} = \hat{\boldsymbol{r}}_{i+1} + \beta_i^* \hat{\boldsymbol{p}}_i$;

Step 3: Compare $\|\boldsymbol{r}_{i+1}\|/\|\boldsymbol{b}\|$ with ε, if $\|\boldsymbol{r}_{i+1}\|/\|\boldsymbol{b}\| < \varepsilon$, jump out from the loop and output $\boldsymbol{x}_{i+1}$, otherwise, go to step 2.

Compared with the traditional CG method in the real number field, the modified BCG method has two advantages:

(1) It calculates only one matrix-vector product, not two like the CG method in each iteration.

(2) It converges about 5-6 times faster than the CG method.

IV. PRECONDITIONED BI-CONJUGATE GRADIENT METHOD

Preconditioned iterative methods [7] obtain the ability of solving linear systems accurately within a few iterations. For large-scale linear systems with symmetric system matrices, an efficient solving scheme is the preconditioned conjugate gradient (PCG) method. Traditional PCG methods are usually available for real linear systems, not for linear complex systems in FEM solution of electromagnetic scattering problems. Therefore, valid iterative methods for complex linear systems are needed. Based on a real preconditioned conjugate gradient algorithm, we design a complex preconditioned bi-conjugate gradient algorithm for solving complex linear systems. The details are as follows:

Step 1: Set $k=0$, input complex matrix $\boldsymbol{A}\in \mathrm{C}^{n\times n}$, preconditioned matrix $\boldsymbol{M}\in \mathrm{C}^{n\times n}$, vector $\boldsymbol{b}\in \mathrm{C}^{n}$, initial vector $\boldsymbol{x}_k\in \mathrm{C}^{n}$ and error criterion ε, compute

$$\boldsymbol{r}_k=\boldsymbol{b}-\boldsymbol{A}\boldsymbol{x}_k,\ z_k=\boldsymbol{M}^{-1}\boldsymbol{r}_k,$$
$$\boldsymbol{p}_{k+1}=z_k,\ \hat{\boldsymbol{r}}_k=\boldsymbol{r}_k^*,$$
$$\hat{\boldsymbol{p}}_{k+1}=\boldsymbol{p}_{k+1}^*,\ \rho_k=(\hat{\boldsymbol{r}}_k,z_k);$$

Step 2: Increase k by 1 and calculate:

$$\boldsymbol{w}=\boldsymbol{A}\boldsymbol{p}_k,\ \alpha_k=\rho_{k-1}/(\hat{\boldsymbol{p}}_k,\boldsymbol{w}),$$
$$\boldsymbol{x}_k=\boldsymbol{x}_{k-1}+\alpha_k\boldsymbol{p}_k,\ \boldsymbol{r}_k=\boldsymbol{r}_{k-1}-\alpha_k\boldsymbol{w},$$
$$\hat{\boldsymbol{r}}_k=\boldsymbol{r}_{k-1}^*-\alpha_k^*\boldsymbol{A}^*\hat{\boldsymbol{p}}_k,\ z_k=\boldsymbol{M}^{-1}\boldsymbol{r}_k,$$
$$\rho_k=(\hat{\boldsymbol{r}}_k,z_k),\ \beta_k=\rho_k/\rho_{k-1},$$
$$\boldsymbol{p}_{k+1}=z_k+\beta_k\boldsymbol{p}_k,\ \hat{\boldsymbol{p}}_{k+1}=z_k^*+\beta_k^*\hat{\boldsymbol{p}}_k;$$

Step 3: Compare $|\rho_k|$ with $|\rho_0|\varepsilon$, if $|\rho_k|>|\rho_0|\varepsilon$, jump out from the loop and output $\boldsymbol{x}_k$, otherwise go to Step 2.

In iterations, the orthogonal vectors and Euclidean products are calculated with the preconditioned matrix $\boldsymbol{M}$ instead of matrix $\boldsymbol{A}$ because the preconditioned matrix $\boldsymbol{M}$ is well-conditioned and easy to be inversed.

V. A COMPLEX INCOMPLETE CHOLESKY FACTORIZATION PRECONDITIONER

The complex system matrix from FEM is always symmetric and sparse, so is the preconditioned matrix. In order that the preconditioned matrix $\boldsymbol{M}$ is easily inversed in simple storing structure, the sparse structure between matrix $\boldsymbol{A}$ and preconditioning matrix $\boldsymbol{M}$ should be the same or approximately the same. In some preconditioned methods [8-10], the sparse structure of preconditioning matrix $\boldsymbol{M}$ is designed by abandoning all possible non-diagonal filling elements (zero-filling mode) during the incomplete factorization. Considering that nonzero elements of preconditioning matrix $\boldsymbol{M}$ and matrix $\boldsymbol{A}$ can be stored in the same sparse database, the zero-filling Cholesky factorization method is used widely as an efficient preconditioner.

If a matrix $\boldsymbol{A}\in \mathrm{C}^{n\times n}$ is symmetric, its incomplete Cholesky factorization formula is written as

$$\boldsymbol{A}=\boldsymbol{L}\boldsymbol{L}^{\mathrm{T}}+\boldsymbol{R}, \tag{2}$$

where the matrix $\boldsymbol{L}$ is a lower triangle matrix and matrix $\boldsymbol{R}$ is a residual matrix [11]. The matrix $\boldsymbol{M}=\boldsymbol{L}\boldsymbol{L}^{\mathrm{T}}$ is defined as a preconditioned matrix. During the incomplete Cholesky factorization, the filling elements of residual matrix $\boldsymbol{R}$ can be designed in advance, so it is easy to ensure the same sparse structure of matrix $\boldsymbol{L}$ as matrix $\boldsymbol{A}$. As a well-condition approximate of matrix $\boldsymbol{A}$, matrix $\boldsymbol{M}$ is the main driving factor for the rapid convergence of preconditioned iterative method.

Based on a real incomplete Cholesky factorization algorithm in [12], a complex incomplete Cholesky preconditioner is proposed by the zero-filling mode. During the complex incomplete Cholesky factorization, some diagonal elements are modified to possess the diagonal predomination of preconditioned matrix. The algorithm detail is expressed as follows.

Input system matrix $\boldsymbol{A}=(a_{ij})_{n\times n}\in \mathrm{C}^{n\times n}$ and output preconditioned matrix $\boldsymbol{M}=\boldsymbol{L}\boldsymbol{L}^{\mathrm{T}}$ (lower triangle matrix $\boldsymbol{L}=(l_{ij})_{n\times n}\in \mathrm{C}^{n\times n}$).

1. $l_{11}=\sqrt{a_{11}}$
2. For $i=2$ to n do

3. If $|a_{i1}| \neq 0$ then $l_{i1} = a_{i1}/l_{11}$
4. End do
5. For $k = 2$ to n do
6. If $|a_{kk}| \geq \sum_{t=1}^{k-1} |g_{kt}|^2$ then $l_{kk} = \sqrt{a_{kk} - \sum_{t=1}^{k-1} |l_{kt}|^2}$,
   else $l_{kk} = a_{kk}$ (modifying diagonal elements)
7. For $i = k+1$ to n do
8. If $|a_{ik}| \neq 0$ then $l_{ik} = \frac{1}{l_{kk}^*}(a_{ik} - \sum_{t=1}^{k-1} l_{it} l_{kt}^*)$
9. End do
10. End do

VI. NUMERICAL EXPERIMENTS

In this section, in order to verify the accuracy and efficiency of the proposed complex preconditioned bi-conjugate gradient algorithm, we implement the algorithm in eight classical experiments.

(1) 2-D scattering model of radar cover, 6-node curve triangle vector element, 6 unknowns in every element, 6532 unknowns in total.

(2) 2-D scattering model of aerofoil, 8-node curve quadrangle vector element, 8 unknowns in every element, 10442 unknowns in total.

(3) 3-D scattering model of nose, 10-node curve tetrahedron vector element, 20 unknowns in every element, 45228 unknowns in total.

(4) 3-D scattering model of rudder, 20-node curve hexahedron vector element, 54 unknowns in every element, 129812 unknowns in total.

(5) 3-D scattering model of elevator, 20-node curve hexahedron vector element, 54 unknowns in every element, 103236 unknowns in total.

(6) 3-D scattering model of leading edge, 8-node curve quadrangle shell vector element, 28 unknowns in every element, 51682 unknowns in total.

(7) 3-D scattering model of trailing edge, 8-node curve quadrangle shell vector element, 28 unknowns in every element, 46844 unknowns in total.

(8) 3-D penetrating model of radome, 20-node curve hexahedron vector element, 48 unknowns in every element, 87762 unknowns in total.

In Table 2, we show storing scales of system matrixes in the above numerical experiments by the fully-sparse storing scheme. The results suggest that the sparse proportion decreases gradually with increasing the scale of system matrix. Therefore, the fully-sparse storing scheme profits the large-scale sparse matrix.

Table 2: Storage scale comparison

Ex	Unknowns	Nonzero elements stored	Sparse proportion (‰)
1	6532	121430	2.846
2	10442	210874	1.934
3	45228	2544691	1.244
4	129812	11762106	0.698
5	103236	7684181	0.721
6	51682	2978082	1.115
7	46844	2701257	1.231
8	87762	6870334	0.892

Note: Sparse proportion is a ratio of nonzero elements stored in all elements.

In Table 3, we compare the computation efficiency of complex preconditioned bi-conjugate gradient (PBCG) method with other iterative methods. All complex linear systems are obtained from the above experiments. The results show that the proposed complex PBCG method converges with much fewer iterations and less time than other methods.

Table 3: Results of different methods ($\varepsilon = 10^{-8}$)

Part I

Ex	CG		ILU		ICCG	
	iters	time	Iters	Time	iters	time
1	1711	27.63	1072	22.06	756	18.23
2	2048	39.45	1557	33.65	1369	30.28
3	7485	153.2	4555	119.3	3728	89.67
4	18772	526.3	11018	371.9	7952	250.4
5	15772	492.5	10774	327.8	6891	213.6
6	8764	177.1	5991	124.3	4012	101.3
7	8027	165.4	4799	121.1	3845	98.25
8	11344	346.8	8912	244.5	6679	194.5

Part II

Ex	BCG		PBCG	
	iters	time	iters	time
1	576	6.41	115	3.07
2	623	9.62	137	4.79
3	2564	28.77	208	6.25
4	6889	106.4	416	17.04
5	5742	98.82	389	15.88
6	2232	35.79	307	11.72
7	2116	33.14	295	10.98
8	4288	65.55	346	12.07

All results are computed with P4 3.0G CPU 512M-memory computer. All programs are developed in FORTRAN90 language.

VII. CONCLUSION

For the purposes of efficient data access and economic data storage in solving sparse linear systems, we proposed a fully-sparse storing scheme that stores only nonzero symmetrical elements. To accelerate the convergence of bi-conjugate gradient method, we developed the complex incomplete Cholesky factorization preconditioner that can improve the ill-condition system matrix. In view of its high efficiency on the large-scale complex linear systems, the complex PBCG method with fully-sparse storing scheme shows great promise as an ideal solver for large-scale electromagnetic computation.

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