Acceleration of Multiple Solution of a Boundary Value Problem Involving a Linear Algebraic System

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Abstract. Multiple solution of a boundary value problem that involves a linear algebraic system is considered. New approach to acceleration of the solution is proposed. The approach uses properly the structure of the linear system matrix. Particularly, location in the right columns and low rows of the matrix for entries, which undergo variation due to the computing in the range of parameters, is used to apply block LU decomposition. Application of the approach is considered on multiple computing of the capacitance matrix by method of moments used in numerical electromagnetics. Expressions for analytic estimation of acceleration are presented. Results of the numerical experiments for solution of 100 linear systems with matrix orders of 1000, 2000, 3000 and different relations of variated and constant entries of the matrix show that using the block LU decomposition for multiple solution of linear algebraic systems can be effective. The speed up as compared to pointwise LU factorization increases (up to 15) for larger number and order of considered systems with lower number of variated entries.

Keywords: method of moments, linear algebraic systems, block LU decomposition, multiple solution.
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INTRODUCTION

Numerical methods are widely used in science and engineering to solve boundary value problems. As opposed to analytical methods that can treat only simple particular structures, the numerical methods are, as a rule, applicable to arbitrary structures, however have considerable computational costs. Unfortunately, it restricts their usage for analysis in range of parameters and global optimization that are often required in practice. Therefore, new developments of numerical methods for accelerated solving boundary value problems are necessary. There are different approaches to do it. Particularly, alongside with modifications in the essence of methods the improvements of separate routines are proposed. Such representative routine is solution of linear algebraic system, to which solution of a boundary problem are often reduced, for example, by Boundary element method. Various methods are used for solution of one linear system, while few of them can effectively accelerate the multiple solution. For example, the iterative BiCGStab (when irregularly located matrix entries vary [1]) and direct block LU decomposition (when diagonal entries in the right lower corner of the matrix vary [2]) methods are used. The first one permits to treat variations of all parameters of a structure, while the second one is limited by permittivity only. However, an iterative solution is approximate by its essence, while block LU decomposition permits to obtain accurate solution. Therefore it is important to extend the use of block LU decomposition for more general cases of parameter variations to accelerate the multiple solution of linear algebraic systems in boundary value problems. The aim of this paper is to consider the possible extensions.

PROPOSED APPROACH

Despite of generality of the proposed approach, which, in general case, can be used with a numerical method reducing the solution of a boundary value problem to the linear algebraic system, be specific, application of the approach is considered on example of the particular case of Boundary element method named as method of moments (MoM) and widely used in numerical electromagnetics. Particularly, we consider the MoM based calculation of capacitance matrix of a configuration of conductors and dielectrics. For the calculations we used the fast and accurate models in available TALGAT software [3]. (Detailed derivation of the models is presented in [4, 5, 6]. The models for brevity are omitted here but can be presented for completeness in extended version of this paper.) Generally, in case of multiple solution of linear algebraic systems the Gauss elimination or pointvise LU factorization are used to solve each of the systems. However, consideration of structure of MoM matrix in the particular model can reveal new opportunities for acceleration of total solution.

For general case of arbitrarily oriented boundaries of conductors and dielectrics (model for 2D configuration is considered in [4]) the MoM matrix has the structure from Figure 1 *a*, schematically showing a location of matrix entries corresponding to conductor (C) and dielectric (D) boundaries. Note that in case of variations of only D-entries the block LU decomposition can be used to accelerate the multiple solution. For particular case of linear and orthogonal boundaries of 2D configuration [5] the MoM matrix has the structure shown in Figure 1 *b*, where the each former block of Figure 1 *a* consists of 4 parts corresponding to boundaries orthogonal to the Y axis (⊥Y) and to the X axis (⊥X). Note that in case of variations of entries located only in the right and low blocks of the matrix the LU decomposition can be also used. Moreover, it can be even more effective, for example, if only ⊥X-entries corresponding to dielectric boundaries (right column and low row in Figure 1 *b*) are varied. At last, similar one is observed for particular case of rectangular and orthogonal boundaries of 3D-configuration [6] shown in Figure 1 *c*, where the each former block of Figure 1 *a* consists of 9 parts corresponding to boundaries orthogonal to the Y axis (⊥Y), Z axis (⊥Z) and X axis (⊥X). Again, in case of variations of entries located only in the right and low blocks the LU decomposition can be also effectively used.

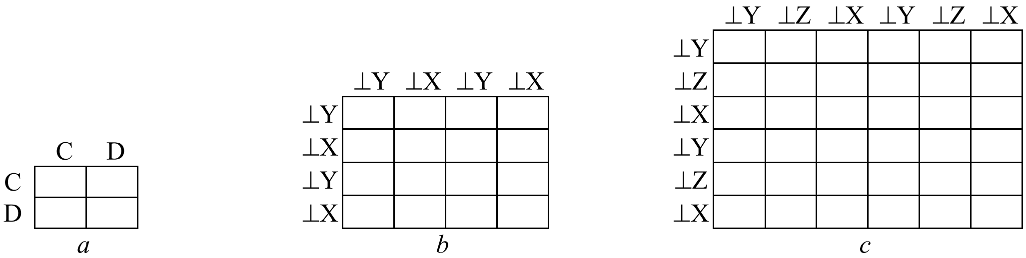

FIGURE 1. Structures of the MoM matix for arbitrary (*a*) and orthogonal orientations of boundaries for 2D (*b*) and 3D (*c*) configurations of conductors and dielectrics

Obviously, a lot of configurations and variations of their parameters exists that permit direct and easy usage of the proposed approach. Particularly, effect of dielectric layers on microstrip line parameters (defined by capacitance calculation) is important in practice [7]. Examples of single and coupled microstrip lines are shown in Figure 2. One can see that all dielectric boundaries of this configuration are orthogonal only to vertical (Y) axes (there are no the dielectric boundaries orthogonal to horizontal (X) axes), while the variation of dielectric cover height (h_C) leads to variation only of one dielectric boundary. Therefore, all variated dielectric ⊥Y-entries of the MoM matrix can be located in right columns and low rows of the matrix. Thus, the LU decomposition can be used in the multiple solution for these configurations.

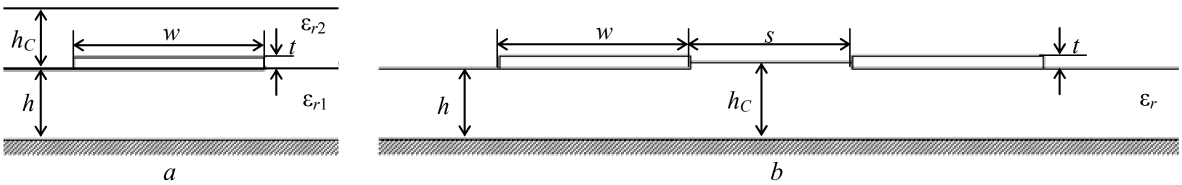

FIGURE 2. Cross sections of single (*a*) and coupled (*b*) microstrip lines illustrating the structure of the MoM matix of Figure 1 *b*

It is worth noting that the above consideration shows that the direct application of the proposed approach can be wide, but it is limited. However, to use it without user concerns about applicability of the approach to the particular case there is way to extend it to any case. Indeed, when a desirable parameter variation is defined by a user, a run of simple software routine can quickly reveal, what entries of matrix are variated. Then, a run of another software routine can properly renumber the subintervals (or subdomains) of each boundary so that all variated entries are located now in right columns and low rows of the matrix. As a result of such "variative renumbering" (being the new step between traditional meshing and matrix filling), we have complete preparation (without user intervention) of a matrix to effective usage of block LU decomposition for arbitrary configuration variations. Moreover, the consequently refined meshing can be used iteratively for additional acceleration. More detailed consideration of the routines is omitted here because it is straightforward and not principal for the proposed approach. However it can be described in extended version of this paper.

BLOCK LU DECOMPOSITION IN MULTIPLE COMPUTATIONS

Consider the block LU decomposition algorithm on the example of a matrix of the form

$$\mathbf{S}=\begin{bmatrix}\mathbf{A} & \mathbf{B}\\ \mathbf{C} & \mathbf{D}\end{bmatrix},$$

where the blocks **A** and **D** are of orders N_A and N_D, respectively (here we use for subscripts the names of blocks **A** and **D**). Then, the block LU decomposition has the following block form [2]

$$\mathbf{S}=\begin{bmatrix}\mathbf{A} & \mathbf{B}\\ \mathbf{C} & \mathbf{D}\end{bmatrix}\Rightarrow\ \mathbf{L}=\begin{bmatrix}\mathbf{I} & \mathbf{0}\\ \mathbf{C}\mathbf{A}^{-1} & \mathbf{I}\end{bmatrix},\mathbf{U}=\begin{bmatrix}\mathbf{A} & \mathbf{B}\\ \mathbf{0} & \mathbf{D}-\mathbf{C}\mathbf{A}^{-1}\mathbf{B}\end{bmatrix}, \tag{1}$$

where **I** is the identity matrix.

One can see from (1), that inverse of matrix **A** must be computed not only once. Therefore, we can replace matrix **S** by its intermediate form (named here as **S'**) that is more appropriate for storage and following usage:

$$\mathbf{S}=\begin{bmatrix}\mathbf{A} & \mathbf{B}\\ \mathbf{C} & \mathbf{D}\end{bmatrix}\Rightarrow\mathbf{S}'=\begin{bmatrix}\mathbf{S}'_{11} & \mathbf{S}'_{12}\\ \mathbf{S}'_{21} & \mathbf{S}'_{22}\end{bmatrix}=\begin{bmatrix}\mathbf{A}^{-1} & \mathbf{A}^{-1}\mathbf{B}\\ \mathbf{C} & \mathbf{D}-\mathbf{C}\mathbf{A}^{-1}\mathbf{B}\end{bmatrix}. \tag{2}$$

Then, in fact the computation steps are following: $\mathbf{S}'_{11}=\mathbf{A}^{-1}$, $\mathbf{S}'_{21}=\mathbf{C}$, $\mathbf{S}'_{12}=\mathbf{S}'_{11}\mathbf{B}$, $\mathbf{S}'_{22}=\mathbf{D}-\mathbf{S}'_{21}\mathbf{S}'_{12}$.

One can see from (2), that for multiple computations a change of block **A** leads to recalculation of matrix **S'**. Computation of the block $\mathbf{S}'_{11}$ (inverse of the block **A**) is the most time consuming. When changing the block **A**, the use of block LU decomposition will be ineffective. However, when changing the blocks **B**, **C**, **D** only, it is necessary recalculate only the matrix **S'** blocks that depend on the changed blocks of matrix **S**. Thus, in case of M computations it is effective for acceleration to compute once the time consuming block $\mathbf{S}'_{11}$ and to make M considerably less expensive computations of blocks $\mathbf{S}'_{12}$ and $\mathbf{S}'_{22}$.

In order to obtain an analytic expression for the resulting acceleration, consider (as in [2]) the ratio (β) of the total time of solving M linear algebraic systems by the original algorithm (based on the pointwise LU factorization) to the time of solving them by the improved algorithm (based on the block LU decomposition). We have

$$\beta=\frac{MT_{LU}}{T_1+(M-1)T_S}\ . \tag{3}$$

where T_{LU} is the time of solving a linear algebraic system by the pointwise LU factorization; T_1 is the time of the first solution, which includes the inversion of the block **A** of order N_A and the subsequent solution of the first linear system; T_S is the time of computing the blocks $\mathbf{S}'_{12}$ and $\mathbf{S}'_{22}$ and of the subsequent solution of the corresponding linear system. It is stipulated that the times of solving a linear system using both the pointwise and block LU factorizations are equal. From (3) it follows that the maximum possible acceleration is given by

$$\beta_{max}=\lim_{M\to\infty}\frac{MT_{LU}}{T_1+(M-1)T_S}=\frac{T_{LU}}{T_S}\ . \tag{4}$$

From (3)–(4) it follows that the larger M the less the acceleration depends on the time of the first solution T_1. Also it is seen that the acceleration is inversely proportional to the time of computing the blocks $\mathbf{S}'_{12}$ and $\mathbf{S}'_{22}$, which is determined mainly by the order of N_D. Thus, for large M and N_A with small N_D, a considerable acceleration of multiple computations can be expected.

NUMERICAL EXPERIMENTS

In numerical experiments we used a personal computer (parallelization was not exploited, i.e. one processor core was busy) with the following parameters: platform – AMD FX(tm)-8350 Eight-Core Processor; processor frequency – 4.01 GHz; memory – 32 Gb; number of cores – 8; operation system – Windows 7x64. Linear algebraic system solutions based on the pointwise LU factorization and block LU decomposition were software implemented. Computations were carried out for the following parameters: N=1000, 2000, 3000; N_D/N=0.001, 0.01, 0.1; M=10, 20, …, 100. Obtained accelerations (β) are presented in Table. One can see that the acceleration exists for all considered cases. This fact confirms that using the block LU decomposition for multiple solution of linear algebraic systems can be effective. The speed up increases (up to 15) for larger number and order of considered systems with lower number of variated entries.

TABLE. Obtained accelerations (β) for M linear algebraic system solutions

N	N_D/N	M									
		10	**20**	**30**	**40**	**50**	**60**	**70**	**80**	**90**	**100**
1000	0.1	1.17	1.68	1.96	2.14	2.26	2.36	2.43	2.50	2.54	2.57
	0.01	1.37	2.58	3.65	4.70	5.60	6.50	7.28	8.03	8.75	9.35
	0.001	1.39	2.74	3.98	5.36	6.65	7.99	9.26	10.56	11.81	13.00
2000	0.1	1.31	1.89	2.22	2.44	2.59	2.69	2.77	2.83	2.90	2.94
	0.01	1.51	2.89	4.16	5.32	6.37	7.34	8.25	9.06	9.87	10.57
	0.001	1.54	3.07	4.59	6.10	7.58	9.06	10.35	11.92	13.38	14.75
3000	0.1	1.35	1.95	2.29	2.52	2.67	2.78	2.88	2.95	2.99	3.04
	0.01	1.55	2.97	4.25	5.44	6.53	7.54	8.48	9.34	10.12	10.87
	0.001	1.59	3.14	4.70	6.30	7.76	9.26	10.78	12.26	13.69	15.17

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