Iterative Application of Boundary Conditions in the Parallel Implementation of the FDFD Method

Michał Rewieński and Michał Mrozowski, *Member, IEEE*

***Abstract*—This letter presents an implementation of the finite difference frequency domain (FDFD) algorithm, based on extending the problem domain and iterative application of boundary conditions, which allows efficient parallel solution of the electromagnetic problems defined over irregular computational domains. The proposed approach applied jointly with implicit representation of the operator matrix and spectral transformations has been used to develop a parallel solver for the open resonator problem, characterized by a nearly optimal speedup of computations.**

***Index Terms*—Boundary conditions, FDFD, parallel computation, resonators.**

I. Introduction

MODELING of large or complex electromagnetic structures in the frequency domain often involves solving sparse matrix problems with the number of unknowns as high as 10^5–10^6. To this end, iterative techniques based on Krylov subspace concept are applied [1]–[3]. These iterative techniques are very attractive as they are also well suited for application in scalable parallel systems which offer multiple processor power and memory resources. Still, in order to obtain good speedup in computations, a parallel algorithm has to satisfy the two key requirements:

1) assure workload balancing among the processors, and
2) minimize the data communication across the processors.

Whether these requirements may be easily satisfied or not depends largely on the properties of the involved operator matrix.

One of the simplest and yet very powerful algorithm which is easy to implement on a parallel system is the finite difference frequency domain (FDFD) method. The standard FDFD algorithm gives a matrix with a highly regular structure. The basic operator can be represented by a few diagonals which is extremely advantageous in the context of parallelization, as e.g., it allows one to maintain almost a perfect workload balancing and extremely low inter-processor communication while performing calculations.

A regular structure of the matrix is spoiled when irregular domains have to be considered. This is because the boundary conditions are a priori included in the matrix, e.g., by eliminating from the matrix representation the elements corresponding to vanishing field components located on the boundaries. As a result the operator matrix looses its purely diagonal structure and becomes a banded matrix. This in turn implies that the parallelization efficiency is frequently deteriorated, due to the increased amount of inter-processor communication and problems with workload balancing.

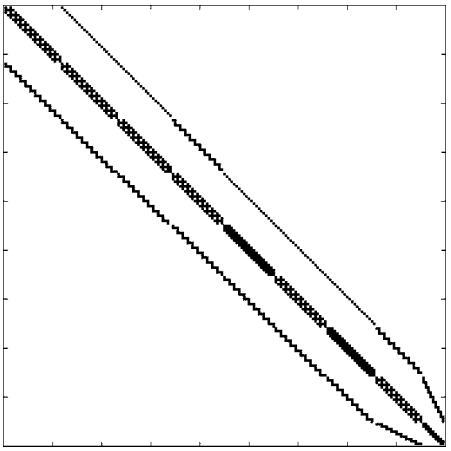

Fig. 1. Pattern of distribution of nonzero elements in the operator matrix for the standard FDFD algorithm.

A typical example of such a situation is the problem of modeling of a hemispherical resonator [4], [5]. For this problem the FDFD projection gives an operator matrix, whose nonzero elements are basically located on 11 diagonals. This regular structure of the matrix is however spoiled by the boundary conditions at the hemispherical part of the boundary (see Fig. 3 for the geometry) because the nodes located inside the metal are removed. This reduces the number of unknowns, but at the same time it disturbs the regular structure. The nonzero elements move toward the main diagonal and the matrix receives a banded structure (cf. Fig. 1). There are still 11 nonzero elements in a row but they are located at various distances from the main diagonal. In the example considered, the upper mirror is spherical, so the matrix becomes very tapered as one moves toward the upper mirror, which deteriorates parallel performance of the numerical solver.

II. Iterative Application of Boundary Conditions

The difficulties associated with parallel performance may be overcome if the computational domain is regularized and the Krylov space iterations characteristic of the sparse solvers used in the FDFD method are implemented so that 1) the operator matrix is not explicitly constructed but rather created on-the-fly

Manuscript received May 15, 2000; revised July 21, 2000. This work was supported by the Polish State Committee for Scientific Research under Contract 8T11D 003 18.

M. Rewieński was with the Faculty of Electronics, Telecommunications and Informatics at Technical University of Gdańsk, 80-952 Gdańsk, Poland. He is now with the Department of Electrical Engineering and Computer Science, Massachusetts Institute of Technology, Cambridge, MA 02139 USA.

M. Mrozowski is with the Faculty of Electronics, Telecommunications and Informatics at Technical University of Gdańsk, 80-952 Gdańsk, Poland (e-mail: mrewiens@mit.edu; mim@pg.gda.pl).

Publisher Item Identifier S 1051-8207(00)08449-X.

and 2) and boundary conditions are applied at each iteration of the solution process.

The proposed scheme may be illustrated for a simplified example of a two-dimensional (2-D) Laplace's operator. Let $S \in R^2$ be an irregular computational domain for our problem. We denote by S' some regular (e.g., rectangular) domain which contains S. Suppose we define a regular FD grid over S' and discretize both the fields and the Laplace operator using this grid. If we apply e.g., a Krylov subspace method, then the information on the problem is passed to the algorithm by repeatedly computing the matrix vector product $\underline{\underline{L}}\underline{v}$, where $\underline{\underline{L}}$ is the projected Laplace's operator and $\underline{v} = [v_{ij}]$ is a given vector containing the iterates of the values of fields at the grid points. In the proposed scheme, assuming homogeneous boundary conditions, the matrix-vector product is computed in the following steps:

Step 1) For $(i, j) \in \{(k, l)\colon (x_k, y_l) \in (S' - S)\}$ we zero the elements v_{ij} of the input vector.

Step 2) We compute $\underline{w} = \underline{\underline{L}}\underline{v}$ by implicitly representing the discrete operator $\underline{\underline{L}}$, i.e., we compute $\underline{w}$ by performing linear operations on vector $\underline{v}$ determined by the formula

$$w_{ij} = \frac{v_{i+1,j} + v_{i-1,j} - 2v_{ij}}{\Delta x^2} + \frac{v_{i,j+1} + v_{i,j-1} - 2v_{ij}}{\Delta y^2} \quad (1)$$

Step 3) We zero the elements w_{ij} of vector $\underline{w}$ for $(i, j) \in \{(k, l)\colon (x_k, y_l) \in (S' - S)\}$.

In steps 1) and 3), we impose the correct boundary conditions by simply zeroing the appropriate vector components, which is due to the particularly simple form of the operator. In case of realistic electromagnetic operators the proposed method of iterative application of boundary conditions is more involved. In fact the FDFD iterations for electromagnetic problems are implemented in a way analogous to the marching-in-time algorithm of the FDTD method [6].

As an example let us present the technique for the problem of the open hemispherical resonator. For the considered structure, assuming the $\exp(-jn\phi)$ variation of the fields in the $\hat{\phi}$ direction, the eigenproblem being solved yields the following form [7]:

$$c^2 \Gamma \nabla \times \overleftrightarrow{\mu}^{-1} \nabla \times \overleftrightarrow{\epsilon}^{-1} \left(\Pi \tilde{D} - \hat{\phi} \frac{jr}{n} \tilde{\nabla} \cdot \tilde{D} \right) = \omega^2 \tilde{D} \quad (2)$$

where $\Gamma[A_r, A_\phi, A_z] = [A_r, A_z]$, $\Pi[A_r, A_z] = [A_r, 0, A_z]$, $\tilde{D} = [D_r, D_z]^T$ is the unknown eigenfunction consisting of two electric flux components and ω is the unknown resonant frequency. Let us consider the discrete version of the problem given above, which may be written as follows:

$$\underline{\underline{L}}_{dh} \underline{\underline{L}}_{he} \underline{\underline{L}}_{ed} \underline{\tilde{D}} = \omega^2 \underline{\tilde{D}} \quad (3)$$

where $\underline{\underline{L}}_{dh}$, $\underline{\underline{L}}_{he}$ and $\underline{\underline{L}}_{ed}$ are appropriate finite difference operators. Vector $\underline{\tilde{D}}$ contains values of the two electric field components D_r and D_z ordered in the following way:

$$\underline{\tilde{D}} = [D_r^{11}, D_z^{11}, \cdots, D_r^{M1}, D_z^{M1}, \cdots, D_r^{MN}, D_z^{MN}] \quad (4)$$

where M and N denote the number of grid points in r and z directions, respectively. If $M < N$, then the above indexing scheme gives a matrix with the narrowest bandwidth, which minimizes the inter-processor communication during computation of the matrix-vector product. In the proposed method, we assume that the problem is defined on Yee's mesh and the elementary finite difference operators are the same throughout the extended, regular computational domain, which includes the cells located inside the metal in the upper mirror. The elementary discrete divergence and rotation operators are identical as those of FDTD. During the computation of the Krylov vectors elementary operators are applied successively from right to left to 2-D discrete field $\underline{\tilde{D}}$. This corresponds to a sequence of linear field transformations

$$\underbrace{\underline{\tilde{D}} \rightarrow \underline{E}}_{\underline{\underline{L}}_{ed}} \underbrace{\rightarrow \omega \underline{H}}_{\underline{\underline{L}}_{he}} \underbrace{\rightarrow \omega^2 \underline{\tilde{D}}}_{\underline{\underline{L}}_{dh}}. \quad (5)$$

The boundary conditions are applied at appropriate stages of these transformations. All electric field components inside metal are zeroed and the electric and magnetic fields for Yee's

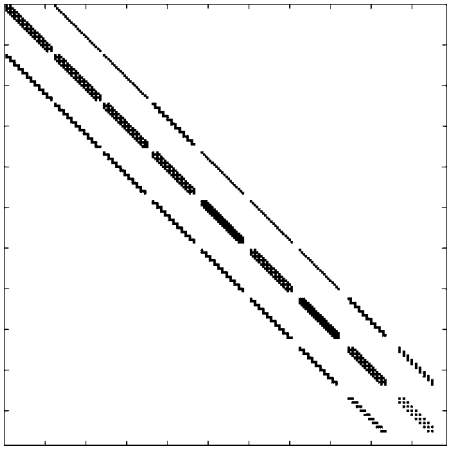

Fig. 2. Pattern of distribution of nonzero elements in the operator matrix for the FDFD algorithm with an extended computational domain.

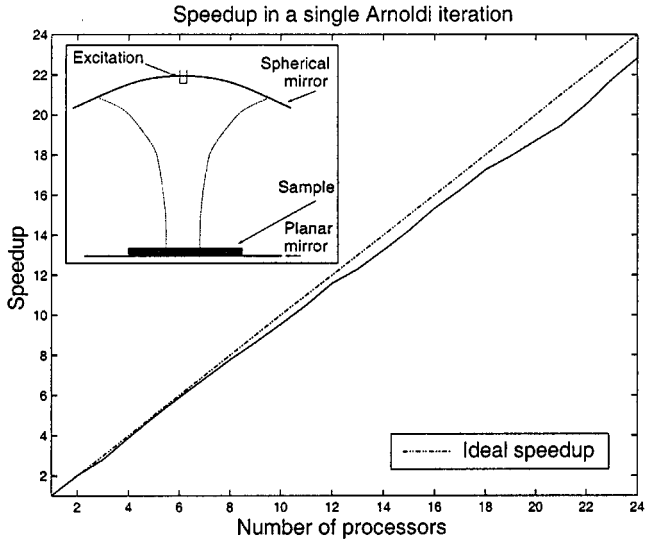

Fig. 3. Speedup in the computations for the parallel solver of the open hemispherical resonator problem in the Cray T3E system. Matrix size $N = 165\,100$.

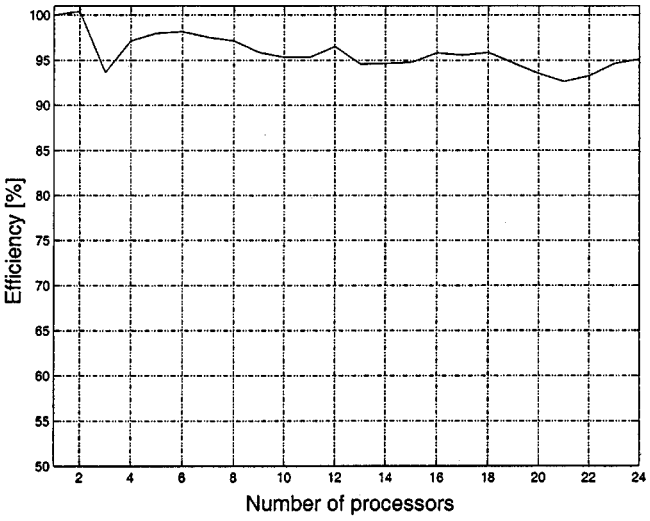

Fig. 4. Efficiency of the parallel solver in the Cray T3E system. Matrix size $N = 165\,100$.

cells crossing the boundary are computed at an appropriate intermediate transformation stage using a conformal algorithm introduced in [6].

During the computation of Krylov subspace, the matrix operator and the operators of boundary conditions are represented implicitly, i.e., the matrix is never constructed. Nevertheless, we may consider the equivalent matrix explicit form of the discretized operator, which has been shown in Fig. 2. The equivalent matrix obtained using the proposed method has a slightly larger size than the explicit matrix obtained with the standard, sequential algorithm still, unlike the other one, it has a regular 11-diagonal structure. This in turn enables one to develop highly efficient parallel code of computing the Krylov vectors characterized by nearly optimal workload balancing and very low inter-processor data communication.

III. Spectral Transformations

The matrix operator obtained with the presented method of treatment of boundary conditions has one disadvantage over the original operator. By including the points located on the boundary of the resonator in the computational domain, we introduce zero eigenvalues to the spectrum of the discrete operator. This deteriorates the convergence of the iterative Krylov subspace methods, such as Arnoldi algorithm, used to solve the discrete eigenproblem. In order to retain fast convergence of the algorithm, we apply spectral transformations, based Chebyshev polynomials [5], [8] and polynomial filtration proposed in [9], which eliminate the zero eigenvalues from the spectrum of the operator.

IV. Performance Results

The presented method of treatment of boundary conditions enabled us to develop a highly efficient parallel code of computing the Krylov subspace (matrix-vector products), characterized by nearly optimal workload balancing and parallel data distribution requiring minimal inter-processor communication. Iterative application of spectral transformations and efficient parallel implementation of the Arnoldi method resulted in a scalable parallel numerical solver for the resonator problem featuring a nearly linear (optimal) speedup, as shown in Fig. 3. The achieved efficiency of the solver, computed as $E = 100\% \cdot nT_n/T_1$, where n is the number of applied processors and T_k is the computation time on k processors, is also very high (cf. Fig. 4). Consequently, the solution time for the open hemispherical resonator problem has been reduced from around 10 h to approximately 20 min.

V. Conclusions

In this letter we have proposed a parallel implementation of the FDFD algorithm, based on iterative application of operators of boundary conditions, implicit operator representation and spectral transformations. Results of performance tests obtained for the problem of modeling of an open hemispherical resonator indicate that the proposed technique may be applied to develop scalable parallel electromagnetic solvers.

Acknowledgment

The authors are grateful to A. Ćwikła and J. Mielewski for providing sequential code of the FDFD solver. All numerical tests presented in this letter have been carried out at the facilities of ICM in Warsaw and TASK in Gdańsk.

References

[1] M. Celik and A. C. Cangellaris, "Simulation of multiconductor transmission lines using Krylov subspace order-reduction techniques," *IEEE Trans. Computer-Aided Design*, vol. 16, pp. 485–496, May 1997.

[2] T. Cwik, D. S. Katz, C. Zuffada, and V. Jamnejad, "The application of scalable distributed memory computers to the finite element modeling of electromagnetic scattering," *Int. J. Numer. Methods Eng.*, vol. 41, pp. 759–776, 1998.

[3] M. Clemens, T. Weiland, and U. van Rienen, "Comparison of Krylov-type methods for complex linear systems applied to high-voltage problems," *IEEE Trans. Magn.*, vol. 34, no. 5, pp. 3335–3338, Sep. 1998.

[4] T. E. Harrington, J. Wosik, and S. A. Long, "Open resonator mode patterns for characterization of anisotropic dielectric substrates for HTS thin films," *IEEE Trans. Appl. Superconduct.*, vol. 7, pp. 1861–1864, Jun. 1997.

[5] A. Ćwikła, J. Mielewski, M. Mrozowski, and J. Wosik, "Accurate full wave analysis of open hemispherical resonators loaded with dielectric layers," *IEEE MTT-S Symp. Dig.*, vol. 3, pp. 1265–1268, 1999.

[6] S. Dey and R. Mittra, "A locally conformal finite-difference time domain (FDTD) algorithm for modeling three-dimensional perfectly conducting objects," *IEEE Microwave Guided Wave Lett.*, vol. 7, pp. 273–275, Sept. 1997.

[7] M. Rewieński, "High performance algorithms for large scale electromagnetic modeling," Ph.D. dissertation, Dept. Electr., Telecommun. Comput. Sci., Technical Univ. Gdańsk, Gdańsk, Poland, Dec. 1999.

[8] J. Mielewski, A. Ćwikła, and M. Mrozowski, "Accelerated FD analysis of dielectric resonators," *IEEE Microwave Guided Wave Lett.*, vol. 8, pp. 375–377, Nov. 1998.

[9] D. C. Sorensen, "Implicit application of polynomial filters in a k-step Arnoldi method," Rice Univ., Dept. Math. Sci., Houston, TX, Tech. Rep. TR90-27, 1990.