

Comparative Analysis of Approaches for High Frequency Electromagnetic Simulation

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Abstract. The efficiency of various numerical approaches are compared for solving 3D electromagnetic boundary value problems (BVPs) in frequency domain. The differential and variational statements in terms of electric field as well as in terms of vector and scalar potentials, with different types of boundary conditions (perfect electrical and magnetic conductor, absorption surfaces, wave ports) are approximated at the non-structured grids by finite volume method (FVM) or finite element methods (FEM). FVM is applied for barycentric Voronoi cells, with computing the local balance matrices and assembling the global matrix of the system of linear algebraic equations (SLAE). In FEM, the scalar and vector basis functions are implemented at the tetrahedral elements. The solutions of obtained non-symmetric indefinite SLAEs are made by different preconditioned iterative processes in Krylov subspaces. The Eisenstat modification of incomplete factorization and various preconditioning matrices are combined with semi-conjugate residual (SCR), BiCGStab and other Krylov algorithms. The results of numerical experiments for the representative set of the model problems are presented and demonstrate performance of the proposed algorithms. Computational technologies include parallelization and using the program tools of Mathematical Kernel Library of Intel (MKL).

1 Introduction

The goal of this paper includes the comparative analysis of the different approaches for numerical solution of the 3D mixed boundary value problems for the system of time-harmonic Maxwell equation, see [1], [2] for example:

$$\begin{aligned}\nabla \times \vec{E} &= -i\omega\dot{\mu}\vec{H}, & \nabla \times \vec{H} &= i\omega\dot{\varepsilon}\vec{E} + \vec{J}, \\ \nabla \cdot (\varepsilon_r \vec{E}) &= \rho/\varepsilon_0, & \nabla \cdot (\mu_r \vec{H}) &= 0.\end{aligned}\tag{1}$$

Here $\varepsilon_r, \dot{\varepsilon}, \varepsilon_0, \mu_r, \dot{\mu}$ are physical parameters of the media, ω is frequency, $\rho, \vec{J}$ are charge and current densities, $\vec{E}$ and $\vec{H}$ are the vector electric and magnetic fields.

For $\rho = 0$ the above system is transformed to complex “electrical” Helmholtz equation

$$\nabla \times \left(\frac{1}{\mu_r} \nabla \times \vec{E} \right) - \varkappa \vec{E} = -ik_0 Z_0 \vec{J},\tag{2}$$

where $\varkappa = k_0^2 \dot{\varepsilon}$, $k_0 = \omega \sqrt{\varepsilon_0 \mu_0}$, $Z_0 = \sqrt{\mu_0 / \varepsilon_0}$, $\dot{\varepsilon}_r = \dot{\varepsilon} / \varepsilon_0$.

The solution of (1) or (2) is defined in open domain Ω with boundary $\Gamma = \bigcup_i \Gamma_i$, under various types of boundary conditions at the perfect electric or magnetic conductor Γ_1, Γ_2 respectively, wave port Γ_3 , and absorption surface Γ_4 :

$$\begin{aligned}\Gamma_1 : \quad \vec{n} \times \vec{E} &= 0, & \Gamma_2 : \quad \vec{n} \times \vec{H} &= 0, \\ \Gamma_3 : \quad \vec{E}_\tau &= \vec{E}_0, & \Gamma_4 : \quad \vec{E}_\tau &= Z_0 \left(\vec{H} \times \vec{n} \right).\end{aligned}\tag{3}$$

Here τ is tangent vector component at the surface with the external normal $\vec{n}$. If we introduce scalar and vector potentials $\vec{B} = \mu_r \vec{H} = \frac{i}{\omega} \nabla \times \vec{A}$, $\vec{E} = \vec{A} + \nabla V$, the equation (2) can be rewritten as follows:

$$\nabla \times \left(\frac{1}{\mu_r} \nabla \times \vec{A} \right) - k_0^2 \epsilon_r \left(\vec{A} + \nabla V \right) = -ik_0 Z_0 \vec{J}. \quad (4)$$

For the problems with piece-wise smooth material properties, the well-known conjugation conditions are given on the internal boundaries additionally.

The classical statements (2), (5) can be reformulated in variational forms, see [3], [4]:

$$\begin{aligned} & \int_{\Omega} \frac{1}{\mu_r} (\nabla \times \vec{E}) \cdot (\nabla \times \vec{\Psi}) d\Omega - \int_S \left(\frac{1}{\mu_r} (\nabla \times \vec{E}) \times \vec{n} \right) \cdot \vec{\Psi} dS - \\ & - \int_{\Omega} \mathfrak{x}(\vec{E} \cdot \vec{\Psi}) d\Omega = \int_{\Omega} (\vec{F} \cdot \vec{\Psi}) d\Omega, \quad \forall \vec{\Psi} \in \mathbb{H}_0^{\text{rot}}, \end{aligned} \quad (5)$$

$$\begin{aligned} & \int_{\Omega} \frac{1}{\mu_r} (\nabla \times \vec{A}) \cdot (\nabla \times \vec{\Psi}) d\Omega - \int_S \left(\frac{1}{\mu_r} (\nabla \times \vec{A}) \times \vec{n} \right) \cdot \vec{\Psi} dS - \\ & - \int_{\Omega} \mathfrak{x}(\vec{A} \cdot \vec{\Psi}) d\Omega - \int_{\Omega} \mathfrak{x}(\nabla V \cdot \vec{\Psi}) d\Omega = \int_{\Omega} (\vec{F} \cdot \vec{\Psi}) d\Omega, \quad \forall \vec{\Psi} \in \mathbb{H}_0^{\text{rot}}, \end{aligned} \quad (6)$$

where $\vec{\Psi}$ are some vector probe functions, $\vec{E} \in H^{\text{rot}}$, $V \in H_0^1(\Omega)$.

The approximations of the above BVPs by FVM or FEM were implemented and investigated in the numerous papers, see [3]–[6] and literature cited there. Also, in these and other articles the big attention is paid to the special algorithms for iterative solution of complex non-Hermitian SLAEs which arise in discretization of original problems.

This paper is organized as follows. In point 2 we describe shortly the approximative FVM and FEM to be applied on the non-structural tetrahedral grids as well as algebraic preconditioned iterative methods in the Krylov subspaces which are used for solution of large sparse SLAEs with non-symmetric indefinite matrices for real variables. In the last section the results of numerical experiments for the representative set of the model problems demonstrate the convergence of different grid solutions and the efficiency of algebraic solvers for the various physical parameters and meshsteps.

2 Approximations and iterative algorithms

We construct the discretization of the considered 3D BVPs on the adaptive non-structured grids with tetrahedral elements, i.e. the vertices and edges of the boundary Γ are the mesh nodes and mesh edges also.

Let $\vec{r}_j, j = 1, 2, 3, 4$, be the vertices of some tetrahedra T , and let $u(e), v(e)$ be the beginning and end points of some edge e in T . In each tetrahedra we introduce the linear basis functions $\mathcal{L}_i$ and vector functions $\vec{W}_e$:

$$\mathcal{L}_i(\vec{r}_j) = \delta_{i,j}, \quad \vec{W}_e = \mathcal{L}_{v(e)} \nabla \mathcal{L}_{u(e)} - \mathcal{L}_{u(e)} \nabla \mathcal{L}_{v(e)}. \quad (7)$$

The unknown vector and scalar functions are presented in the form

$$\vec{E} = \sum u_i^E \vec{W}_i, \quad \vec{A} = \sum u_i^A \vec{W}_i, \quad V = \sum u_i^V \mathcal{L}_i \quad (8)$$

where the coefficients u_i^E , for example, are sought from the resulting finite dimensional approximation of (5):

$$\sum_i u_i^E \left[\int_{\Omega} \frac{1}{\mu_r} (\nabla \times \vec{\Psi}_i) \cdot (\nabla \times \vec{\Psi}_j) d\Omega - \int_S \left(\frac{1}{\mu_r} (\nabla \times \vec{\Psi}_i) \times \vec{n} \right) \cdot \vec{\Psi}_j dS - \int_{\Omega} \varkappa (\vec{\Psi}_i \cdot \vec{\Psi}_j) d\Omega \right] = \int_{\Omega} (\vec{F} \cdot \vec{\Psi}_j) d\Omega, \quad (9)$$

The similar relations for each j -th grid edge can be written for $\vec{A} - V$ variational statement (7). The relations (8), (9) define SLAE

$$A^E u^E = f^E, \quad A^E = \{A_{i,j}^E\}, \quad u^E = \{u_i^E\}, \quad f^E = \{f_i^E\}, \quad (10)$$

which dimension N_e equals to the number of mesh edges. The entries of matrix $A_{i,j}^E = S_{i,j} - M_{i,j}$ and vector entries f_i^E are defined via integrals on the finite elements, see [4]:

For the potential statement SLAE can be written in the following form, see [7]:

$$A^{AV} u \equiv \begin{bmatrix} I \\ G^T \end{bmatrix} \cdot [A^E] \cdot \begin{bmatrix} I & G \end{bmatrix} \cdot \begin{bmatrix} u^A \\ u^V \end{bmatrix} = \begin{bmatrix} I \\ G^T \end{bmatrix} \cdot [f^E] \equiv f^{AV}, \quad (11)$$

where identity matrix I and subvector u^A have order N_e , the dimension of subvector u^V equals to the number of nodes N_n , and $G = \{g_{i,j}\} \in R^{N_e, N_n}$ is incident “edge-node” matrix: $g_{i,j} = -1$ or 1 if j is node number of the beginning or end vertex of the i -th mesh edge respectively, and $g_{i,j} = 0$ otherwise.

The finite volume approximation of complex Helmholtz equation

$$-\Delta E + \mu_r \varkappa E = 0, \quad (12)$$

which is derived for the uniform media by means of relation $\text{rot rot} = -\Delta + \text{grad div}$ is made using barycentric Voronoi cells on the same non-structured tetrahedral grid, see [6]. In the case of piecewise constant material properties, the conjugation conditions on the internal boundaries are satisfied automatically in FVM approach.

The iterative solution of SLAE $Au = f$, $A = D - L - U$, where D , $-L$ and $-U$ are diagonal, low and upper triangular parts of A , is made by preconditioned Krylov methods. In particular, we use preconditioning matrix

$$B = (G + L)G^{-1}(G + U), \quad G = \frac{1}{\theta}D, \quad (13)$$

where θ is iterative relaxation parameter, and B can be presented in the factorized form, see [7]:

$$B = L_B U_B, \quad L_B = (G - L)G^{-1/2}, \quad U_B = G^{-1/2}(G - U). \quad (14)$$

Then the efficient Eisenstat modification of two side preconditioning can be realized as follows:

$$\bar{A}\bar{u} = L_B^{-1} A U_B^{-1} U_B u = L_n^{-1} f \equiv \bar{f}, \quad \bar{u} = U_B u. \quad (15)$$

The advantage of such approach consists in the fast multiplication of some vector by matrix $\bar{A}$.

The iterative solution of preconditioned SLAE (15) is made by various Krylov’s methods: conjugate gradient (CG, for symmetric case), biconjugate gradient (BiCG), biconjugate gradient stabilized (BiCGStab) and semi-conjugate residual (SCR), see [7]. Let us remark that the complex SLAEs were transformed to real non-symmetric form.

3 Numerical experiments

The efficiency of the described algorithms is demonstrated by the results of numerical experiments for three test problems (wave guides) with known exact solutions. The computational domain Ω is parallelepiped $0 < x < 72$, $0 < y < 34$, $0 < z < 200$. The surface $z=200$ is wave port with boundary condition $\vec{E} = \vec{e}_y \sin(\frac{\pi x}{72})$, and the rest boundary surfaces are perfect electric conductor. The frequency is $\omega = 6\pi GHz$.

Test 1 includes uniform real parameters $\varepsilon_r = \mu_r = 1$. In the Test 2 the values $\varepsilon_r = 5$ for $0 < z < 100$ and $\varepsilon_r = 1$ for $100 < z < 200$ ($\mu_r = 1$ everywhere in Ω). The third test corresponds to complex parameters $\varepsilon_r = 1 - 0.1i$, $\mu_r = 1$.

The computations were made under double precision real arithmetics at the uniform grid with the number of parallelepipeds $N_p = 16^3, 32^3, 64^3$ which were divided into 6 tetrahedrals. The stopping criteria was chosen for the iterative residual norm $\|r\| \leq \|f\| \cdot 10^{-7}$. The implementation of the iterative solvers was made for conventional compressed sparse row matrix format, see [8].

Table 1 demonstrates the maximum error ΔE for three test problems, obtained by FVM and FEM on the different grids. In FEM approximations, the accuracy is approximately the same for $\vec{E}$ and A-V statement.

N_p	Test 1		Test 2		Test 3	
	<i>FEM</i>	<i>FVM</i>	<i>FEM</i>	<i>FVM</i>	<i>FEM</i>	<i>FVM</i>
16^3	$7.1 \cdot 10^{-1}$	$1.6 \cdot 10^0$	$2.6 \cdot 10^{-1}$	$1.0 \cdot 10^0$	$6.7 \cdot 10^{-1}$	$1.7 \cdot 10^{-1}$
32^3	$2.7 \cdot 10^{-1}$	$2.8 \cdot 10^{-1}$	$1.4 \cdot 10^{-1}$	$5.5 \cdot 10^{-1}$	$3.1 \cdot 10^{-1}$	$4.1 \cdot 10^{-2}$
64^3	$1.1 \cdot 10^{-1}$	$6.4 \cdot 10^{-2}$	—	$7.9 \cdot 10^{-2}$	$1.6 \cdot 10^{-1}$	$1.0 \cdot 10^{-2}$

Table 1: The errors of numerical solution

The Table 2 demonstrates the number of iterations for preconditioned BiCGStab algorithm which are required for solving three test problems at different grids for FVM and FEM approximations. In FEM approach, the A-V formulations (11) was solved. For "electric" SLAE (10) the numbers of iterations are considerably bigger.

N_p	Test 1		Test 2		Test 3	
	<i>FEM</i>	<i>FVM</i>	<i>FEM</i>	<i>FVM</i>	<i>FEM</i>	<i>FVM</i>
16^3	173	53	1169	225	242	112
32^3	402	96	2240	356	509	216
64^3	—	154	—	531	1544	395

Table 2: Number of iterations for different approaches

In the Table 3 we present the computational resources which are necessary for solving Test 3 by iterative SCR method (for A-V variables in FEM statement (6), (11)) and direct PARDISO solver from MKL [8]. Here N means the order of the SLAEs for different grids, T_1 and T_4 are execution times in seconds for one- and four-threads parallel implementations under OpenMP system, and MemGB is the required volume of memory in gigabyte. For 64^3 grid, the PARDISO solver fails because of memory deficit. Let us remark, that in the last experiments the implementation of SCR solver was done by using SPARS BLAS computational tools from MKL. This technology helps to save code execution time about 50%.

The comparative analysis of the presented results and many others numerical experiments allows to make the following conclusions:

Grid	N	SCR				Pardiso		
		n	T_1, sec	T_4, sec	$MemGB$	T_1, sec	T_4, sec	$MemGB$
16^3	59582	216	15.4	13.4	0.28	15.6	6.7	0.44
32^3	50009	411	664	495	3.73	865	302	5.78
64^3	4096766	988	—	17844	47.6	—	—	> 64

Table 3: Test 3: computational resources for different solvers

- the FVM and FEM approaches provide approximately the same accuracy for considered test problems, including complex and piece-wise constant material properties, but the order of convergence for $h \rightarrow 0$ is the first one for FEM and the second one for FVM;
- in FVM case the algebraic properties of SLAE are better considerably which help to obtain more fast iterative solution;
- direct solver PARDISO is really competitive for relatively small SLAEs, but it fails for the very large orders;
- the variational A-V statement has the considerable advantage, compare to FVM for $\vec{E}$ formulation, because of better algebraic properties of SLAE.

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