A Numerical Study of Iterative Substructuring Method for Finite Element Analaysis of High Frequency Electromagnetic Fields

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Abstract

This paper describes iterative methods for the high frequency electromagnetic analysis using the finite element method of Maxwell equations including displacement current. The conjugate orthogonal conjugate gradient method has been widely used to solve a complex symmetric system. However, the conventional method suffers from oscillating convergence histories in large-scale analysis. In this paper, to solve large-scale complex symmetric systems arising from the formulation of the E method, an iterative substructuring method like the minimal residual method is presented, and the performance of the convergence of the method is evaluated by numerical results. As the result, the proposed method shows a stable convergence behavior and a fast convergence rate compared to other iterative methods.

Keywords: Iterative substructuring method, iterative methods, minimal residual method, complex symmetric systems

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1. Introduction

The electromagnetic field simulation in the range of several megahertz to several gigahertz has high demand for industrial and medical applications. The finite element method (FEM) with the formulation of the $\boldsymbol{E}$ method has been used to solve the vector wave equations in high frequency electromagnetic problems. However, the iterative method for solving such finite element equation is known for having bad convergence. By increasing problem size with increasingly complex shape, the convergence is deteriorating further. Therefore, solving large-scale problems efficiently on the parallel computer is a crucial issue, and both a robust convergence for increasing problem size and a scalable parallel efficiency is in great demand [1][2][3]. For the high frequency electromagnetic field analysis, the finite element formulation of the $\boldsymbol{E}$ method yields a large-scale complex symmetric linear system. To solve this systems, the conjugate orthogonal conjugate gradient (COCG) method [4] with the shifted incomplete Cholesky preconditioning has been widely used. However, for the FEM with arbitrary and complex unstructured mesh, the incomplete Cholesky preconditioner has difficulty obtaining the high performance of both parallel efficiency and convergence. Although the multigrid method is well known as the fast iterative method, it faces the difficult problem to solve a large-scale coarse problem in the large-scale analysis.

As an efficient parallel computing method for large-scale finite element analysis (FEA), we have been studying the iterative substructuring method. The iterative substructuring method form is known as the domain decomposition method (DDM) based on the iterative method [5]. The DDM is expected to obtain scalable parallel efficiency on the distributed memory parallel computers [6]. The DDM was applied to large-scale FEA of structural mechanics [7], heat transfer [8], and nonlinear magnetostatic problems with the magnetic vector potential $\boldsymbol{A}$ as an unknown function [9][10][11]. Furthermore, the DDM algorithm for the high frequency electromagnetic problems based on the formulation of the $\boldsymbol{E}$ method was developed [12], and successfully solve a 100 million complex degrees of freedom problem [13][14]. The DDM is also expected to get fast convergence by effective preconditioners such as the balancing domain decomposition (BDD) [15] and the balancing domain decomposition based on constraints (BDDC) [16]. The finite element tearing and interconnecting (FETI) method [17] and the dual-primal FETI (FETI-DP) method [18], which are the dual method of BDD and BDDC respectively, are also well-known DDM algorithm. However, the iterative methods for the high frequency electromagnetic problems is not fully established. Therefore, this paper focuses on the iterative methods for the DDM algorithm.

In the non-overlapping DDM, the whole analysis domain is decomposed into subdomains, and the problem to be solved is also decomposed into subdomain-interior (subdomain) problems and a subdomain-interface (interface) problem. The iterative substructuring method solves the interface problem using the iterative methods with solving subdomain problems, which mean to perform FEA in each subdomain. In the high frequency electromagnetic field analysis with the finite element formulation of the $\boldsymbol{E}$ method, the interface problem and the subdomain problems are also complex symmetric. Hence, the COCG method can be used to solve the interface problem. However, since that formulation leads to the ill-conditioned problem, the COCG method shows oscillating residual norm histories, and suffers from very slow convergence in the large-scale analysis. On the other hand, the conjugate orthogonal conjugate residual (COCR) method, which extends the conjugate residual method for Hermitian linear systems to complex symmetric linear systems, is expected to obtain smoothed convergence behavior [19]. The iterative substructuring method based on the COCR method was applied to the large-scale FEA of the high frequency electromagnetic fields and improved convergence compared with the COCG method [20], however, its convergence behavior remain oscillating tendency.

In this paper, an iterative substructuring method based on a MINRES-like_CS method based on computational procedures of the minimal residual (MINRES) method [21] is presented, and the performance of the convergence of the method is evaluated by numerical results. The formulation of the high frequency electromagnetic problems is described in Section 2. The iterative substructuring method with the iterative methods is discussed in Section 3. Section 4 shows some numerical examples.

2. Finite Element Formulation

Vector wave equations. Let Ω be a domain with the boundary $\partial\Omega$. The vector wave equations which describe an electromagnetic field with single angular frequency ω are derived from Maxwells equations containing the displacement current. The vector wave equations describing an electric field $\boldsymbol{E}$ are given by (1) and (2) using the current density $\boldsymbol{J}$ and the electric field $\boldsymbol{E}$, and assigning j as an imaginary unit

$$\mathrm{rot}\left(\frac{1}{\mu}\mathrm{rot}\boldsymbol{E}\right) - \omega^2\varepsilon\boldsymbol{E} = j\omega\boldsymbol{J} \quad \text{in } \Omega, \tag{1}$$

$$\boldsymbol{E} \times \mathrm{n} = 0 \quad \text{in } \partial\Omega, \tag{2}$$

$$\boldsymbol{J} = \sigma\hat{\boldsymbol{E}}. \tag{3}$$

In (1) and hereafter, rot is the infinitesimal rotation of a 3-dimensional vector field, and described as follows.

$$\mathrm{rot}\boldsymbol{E} = \left(\frac{\partial E_z}{\partial y} - \frac{\partial E_y}{\partial z}\right)e_x + \left(\frac{\partial E_x}{\partial z} - \frac{\partial E_z}{\partial x}\right)e_y + \left(\frac{\partial E_y}{\partial x} - \frac{\partial E_x}{\partial y}\right)e_z, \tag{4}$$

where $\boldsymbol{E} = (E_x, E_y, E_z)$ is a vector field and e_x, e_y, e_z are the unit vector for the x, y, z axes.

Permittivity and permeability are given by $\varepsilon = \varepsilon_0\varepsilon_r$ and $\mu = \mu_0\mu_r$ respectively, where ε_0 denotes vacuum permittivity, ε_r relative permittivity, μ_0 vacuum permeability, and μ_r relative permeability. In this formulation, the permittivity becomes complex permittivity $\varepsilon = \varepsilon_0\varepsilon_r = \varepsilon_0\varepsilon_r^{'} + \sigma/j\omega$. The electric field $\hat{\boldsymbol{E}}$ on known points is substituted into (1) by (3), where the electrical conductivity is denoted as σ. By solving (1) with imposing the boundary condition of (2), we calculate the electric field $\boldsymbol{E}$. The magnetic field $\boldsymbol{H}$ is then calculated from the electric field $\boldsymbol{E}$ as post-processing using Faraday's law of induction, which is expressed by

$$\mathrm{rot}\boldsymbol{E} - j\omega\mu\boldsymbol{H} = 0. \tag{5}$$

Finite element discretization. Next, we describe the finite element discretization. Let us decompose Ω into an union of tetrahedra. $\boldsymbol{E}_h$ is an electric field approximated by the Nédélec elements [22][23], and $\boldsymbol{J}_h$ is an electric current density approximated by the conventional piecewise linear tetrahedral elements. As a result, we have the finite element approximation

$$\iiint_\Omega \mathrm{rot}\boldsymbol{E}_h \cdot \frac{1}{\mu}\mathrm{rot}\boldsymbol{E}_h^* dv - \omega^2 \iiint_\Omega \varepsilon \boldsymbol{E}_h \cdot \boldsymbol{E}_h^* dv = j\omega \iiint_\Omega \boldsymbol{J}_h \cdot \boldsymbol{E}_h^* dv, \quad (6)$$

where $\boldsymbol{E}_h^* \times \mathrm{n} = 0 \quad on\ \partial\Omega$.

3. Iterative substructuring for complex symmetric system

Reduced system. Firstly, we describe the DDM algorithm [10][13]. Let us denote the finite element equation (6) by the matrix form

$$\boldsymbol{K}\boldsymbol{u} = \boldsymbol{f}, \quad (7)$$

where $\boldsymbol{K}$ denotes complex and symmetric matrix, $\boldsymbol{u}$ the unknown vector, and $\boldsymbol{f}$ the known vector.

The polyhedral domain Ω is partitioned into N non-overlapping subdomains

$$\Omega = \bigcup_{i=1}^{N} \Omega^{(i)}, \quad (8)$$

where the superscript (i) corresponds to the subdomain $\Omega^{(i)}$. By reordering, the complex symmetric linear system (7) is rewritten by

$$\begin{bmatrix} \boldsymbol{K}_{II} & \boldsymbol{K}_{IB} \\ \boldsymbol{K}_{IB}^T & \boldsymbol{K}_{BB} \end{bmatrix} \begin{bmatrix} \boldsymbol{u}_I \\ \boldsymbol{u}_B \end{bmatrix} = \begin{bmatrix} \boldsymbol{f}_I \\ \boldsymbol{f}_B \end{bmatrix}, \quad (9)$$

where

$$\boldsymbol{K}_{II} = \begin{bmatrix} \boldsymbol{K}_{II}^{(1)} & & 0 \\ & \ddots & \\ 0 & & \boldsymbol{K}_{II}^{(N)} \end{bmatrix}, \boldsymbol{K}_{IB} = \begin{bmatrix} \boldsymbol{K}_{IB}^{(1)}\boldsymbol{R}_B^{(1)} \\ \vdots \\ \boldsymbol{K}_{IB}^{(N)}\boldsymbol{R}_B^{(N)} \end{bmatrix}$$

$$\boldsymbol{K}_{BB} = \sum_{i=1}^{N} \boldsymbol{R}_B^{(i)T}\boldsymbol{K}_{BB}^{(i)}\boldsymbol{R}_B^{(i)}$$

$$\boldsymbol{f}_I = \sum_{i=1}^{N} \boldsymbol{R}_I^{(i)T} \boldsymbol{f}_I^{(i)}, \boldsymbol{f}_B = \sum_{i=1}^{N} \boldsymbol{R}_B^{(i)T} \boldsymbol{f}_B^{(i)},$$

where the subscripts I and B correspond to unknowns in the interior of subdomains and on the interface boundary, respectively. $\boldsymbol{R}_I^{(i)}$ and $\boldsymbol{R}_B^{(i)}$ are the Boolean matrix to map the global degrees of freedom (DOF) of to local DOF.

Using the block Cholesky factorization, a coefficient matrix of (9) can be expressed by

$$\boldsymbol{K} = \begin{bmatrix} \boldsymbol{I}_I & 0 \\ \boldsymbol{K}_{IB}^T \boldsymbol{K}_{II}^{-1} & \boldsymbol{I}_B \end{bmatrix} \begin{bmatrix} \boldsymbol{K}_{II} & 0 \\ 0 & \boldsymbol{S} \end{bmatrix} \begin{bmatrix} \boldsymbol{I}_I & \boldsymbol{K}_{II}^{-1} \boldsymbol{K}_{IB} \\ 0 & \boldsymbol{I}_B \end{bmatrix}, \tag{10}$$

where

$$\boldsymbol{S} = \sum_{i=1}^{N} \boldsymbol{R}_B^{(i)T} \left(\boldsymbol{K}_{BB}^{(i)} - \boldsymbol{K}_{IB}^{(i)T} \left(\boldsymbol{K}_{II}^{(i)} \right)^{-1} \boldsymbol{K}_{IB}^{(i)} \right) \boldsymbol{R}_B^{(i)} \tag{11}$$

is the Schur complement matrix, $\boldsymbol{I}_I$ and $\boldsymbol{I}_B$ are corresponding identity matrices. Using (10), (9) leads to two linear systems

$$\boldsymbol{S}\boldsymbol{u}_B = \boldsymbol{g}, \tag{12}$$

$$\boldsymbol{K}_{II}^{(i)} \boldsymbol{u}_I^{(i)} = \boldsymbol{f}_I^{(i)} - \boldsymbol{K}_{IB}^{(i)} \boldsymbol{R}_B^{(i)} \boldsymbol{u}_B, i = 1, ..., N, \tag{13}$$

where

$$\boldsymbol{g} = \sum_{i=1}^{N} \boldsymbol{R}_B^{(i)T} \left(\boldsymbol{f}_B^{(i)} - \boldsymbol{K}_{IB}^{(i)T} \left(\boldsymbol{K}_{II}^{(i)} \right)^{-1} \boldsymbol{f}_I^{(i)} \right). \tag{14}$$

(12) is called the interface problem, (13) are the subdomain problems. In this paper, the interface problem is solved by the iterative methods, and then subdomain problems are solved by a direct solver. Each subdomain problem is solved by a sequential direct solver, and solving (13) are performed in subdomain-wise parallel. In here, solving (12) by the Krylov subspace methods require the multiplicatoin of the Schur complement matrix and a vector at each iteration, and it is a similar calculation solving (13) as can be seen from the form of (11). Therefore, from a viewpoint of the computation cost, solving (13) represent only one iteration count of solving (12).

Since the interface problem is also complex symmetric linear system using our finite element formulation, the COCG method have been widely used so far.

The COCG method is relatively small amount of working memory and computational cost per iteration one of the iterative methods for non-Hermitian matrix. On the other hand, the COCR method requires similar working memory and computational cost to the COCG method, and is expected to show smooth convergence behavior compared with the COCG method. However, these methods show oscillating convergence histories, and then suffer from slow convergence in large-scale analysis. Hence, we consider other iterative methods for the iterative substructuring method. To solve large-scale problems efficiently, we prefer iterative methods require similar working memory and computational cost per iteration to the COCG method, in other words, every iteration involves only one vector and coefficient matrix multiplication.

The QMR_SYM method. The quasi-minimal residual (QMR) method [24] has been developed to improve the oscillations in the residual of the bi-conjugate gradient method. For complex symmetric systems, the QMR_SYM method, which is is symmetric version of the QMR method, has been developed [25]. For a comparison purpose, the QMR_SYM is employed to solve the interface problem.

A MINRES-like_CS method. To obtain even more smooth convergence in solving (12), we suggest to use the MINRES method. The MINRES method is typically used for solving symmetric indefinite systems, on the other hand, (12) is the complex symmetric system. Thus, as a variant MINRES method, a MINRES-like_CS method is presented. The MINRES-like_CS uses computation procedures of the MINRES method, which is for real symmetric system, to complex symmetric system. At this paper, the method does not guarantee that the residual decrease monotonically, but is expected to obtain smooth convergence.

The iterative substructuring method based on the preconditioned MINRES-like_CS method can be summarized as follows.

(i) Give initial values

$$\boldsymbol{u}_B^0 = 0$$

$$\boldsymbol{w}^{-1} = 0, \sigma^0 = 0, \gamma^0 = 1, \boldsymbol{w}^0 = 0, \boldsymbol{v}^0 = 0$$

(ii) Reduce the original system to the interface system and compute the residual vector

$$\boldsymbol{v}^1 = \boldsymbol{g} - \boldsymbol{S}\boldsymbol{u}_B^0$$

(iii) Compute the preconditioned vector

$$\text{solve } \boldsymbol{M}\boldsymbol{q}^1 = \boldsymbol{v}^1$$

(iv) Compute scalar values including reference norm to check convergence

$$\beta^1 = \sqrt{(\bar{\boldsymbol{v}}^1, \boldsymbol{q}^1)}$$

$$\eta^1 = \beta^1, \gamma^1 = 1, \sigma^1 = 0$$

$$rnorm^0 = \|\boldsymbol{v}^1\|$$

(v) For $n = 0, 1, \cdots$, repeat following computation until $rnorm^n / rnorm^0 < \delta$

$$\boldsymbol{v}^n = \boldsymbol{v}^n / \beta^n, \boldsymbol{q}^n = \boldsymbol{q}^n / \beta^n$$

$$\boldsymbol{s}^n = \boldsymbol{S}\boldsymbol{q}^n$$

$$\alpha^n = (\bar{\boldsymbol{s}}^n, \boldsymbol{q}^n)$$

$$\boldsymbol{v}^{n+1} = \boldsymbol{s}^n - \alpha^n \boldsymbol{v}^n - \beta^n \boldsymbol{v}^{n-1}$$

$$\text{solve } \boldsymbol{M}\boldsymbol{q}^{n+1} = \boldsymbol{v}^{n+1}$$

$$\beta^{n+1} = \sqrt{(\bar{\boldsymbol{v}}^{n+1}, \boldsymbol{q}^{n+1})}$$

$$\delta = \gamma^n \alpha^n - \gamma^{n-1} \sigma^n \beta^n, \rho_1 = \sqrt{(\delta)^2 + (\beta^{n+1})^2},$$

$$\rho_2 = \sigma^n \alpha^n + \gamma^{n-1} \gamma^n \beta^n, \rho_3 = \sigma^{n-1} \beta^n,$$

$$\gamma^{n+1} = \delta / \rho_1, \sigma^{n+1} = \beta^{n+1} / \rho_1$$

$$\boldsymbol{w}^n = \left(\boldsymbol{q}^n - \rho_3 \boldsymbol{w}^{n-2} - \rho_2 \boldsymbol{w}^{n-1}\right) / \rho_1$$

$$\boldsymbol{u}_B^n = \boldsymbol{u}_B^{n-1} + \gamma^{n+1} \eta^n \boldsymbol{w}^n$$

$$rnorm^n = |\sigma^{n+1}| rnorm^{n-1}$$

$$\eta^{n+1} = -\sigma^{n+1} \eta^n$$

(vi) Compute approximations of subdomain interior

$$\text{solve } \boldsymbol{K}_{II} \boldsymbol{u}_I^n = \boldsymbol{f}_I - \boldsymbol{K}_{IB} \boldsymbol{u}_B^n$$

In the above MINRES-like_CS algorithm, $\boldsymbol{M}$ is the preconditioning matrix, $(\boldsymbol{x}, \boldsymbol{y}) = \sum_{i=1}^{m} \bar{x}_i y_i$ an inner product of complex vectors $\boldsymbol{x}$ and $\boldsymbol{y}$, $\| \cdot \|$ the Euclidean norm, and δ a positive constant as the convergence criterion.

Henceforth, we describe the iterative substructuring method based on the COCG method, the COCR method, the QMR_SYM method, or the MINRES-like_CS method as the DDM-COCG method, the DDM-COCR method, the DDM-QMR_SYM method, or the DDM-MINRES-like_CS method, respectively.

A simplified diagonal-scaling preconditioner. In solving (12), it is difficult to construct the diagonal-scaling preconditioner, which is the most popular preconditioning technique, because Schur complement matrix is not constructed explicitly in general implementation. Therefore, the diagonal of $\boldsymbol{K}_{BB}$ is used instead of $\boldsymbol{S}$, and it is called a simplified diagonal scaling preconditioner.

4. Numerical experiments

A benchmark model. A reentrant-type cavity resonator model is used to evaluate performances of convergence of iterative substructuring methods. The cavity has a diameter of 1.90 and a height of 1.45. In this analysis, the dielectric phantom of the shape of a disk with specific dielectric constant $\varepsilon_r = 80$ and electric conductivity $\sigma = 0.52$ is placed, and the resonance state is investigated. This problem is one of the benchmark problems defined as Testing Electromagnetic Analysis Method Workshop Problem 29 (TEAM29) [26]. The analysis model is shown in Fig. 4. The boundary condition of (2) was applied at the external boundary, and the electric field was given in the antenna. Table 1 shows the number of elements n_e, nodes n_d, and complex DOF n_{cdof} using the $\boldsymbol{E}$ method and the Nédélec elements.

Performance evaluation. We compare convergence behavior of the interface problem between different iterative methods for the interface problem. As the preconditioner, a simplified diagonal scaling preconditioner is used. Convergence criterion δ is 10^{-7}. All computation of the benchmark model was performed by

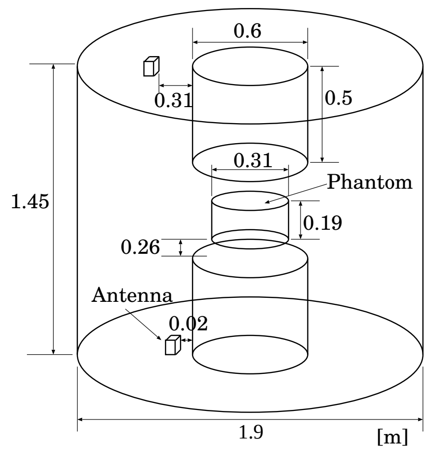

Figure 1: TEAM29 model

Table 1: Mesh information of the TEAM29 model

	n_e	n_d	n_{cdof}
TEAM29(small)	108,595	154,791	0.1 million
TEAM29(large)	17,367,244	23,213,252	20 million

the supercomputer consisting of the Fujitsu PRIMEHPC FX100 at Information Technology Center, Nagoya University.

Firstly, computational performances in the case of solving the small mesh of TEAM29 are evaluated using 32 cores of one computing node. The number of subdomains N is 640. As shown in Table 2, the iteration count and the computation time of four methods are similar extent. In here, $log_{10}\frac{\|\boldsymbol{g}-\boldsymbol{S}\boldsymbol{u}_B^n\|}{\|\boldsymbol{g}-\boldsymbol{S}\boldsymbol{u}_B^0\|}$ in the table is a decadic logarithm of relative true residual norm, means to have enough precision corresponding to $log_{10}\delta$. Fig. 4 shows that DDM-QMR_SYM and DDM-MINRES-like_CS improved oscillating convergence compared to both DDM-COCG and DDM-COCR.

Next, a large-scale analysis with about 20 million complex DOF is demonstrated using 384 cores of 12 computing nodes. The number of subdomains N is 98,304. Table 3 and Fig. 4 shows computational performances and convergence histories, respectively. From these results, DDM-MINRES-like_CS is the fastest method, and successfully reduced both the iteration count and the computation time by about 70% compared to COCG.

Table 4 shows results of the number of iterations in various number of subdomains. As shown in the table, DDM-MINRES-like_CS achieve the fastest convergence rate without dependence on the number of subdomains.

Fig. 4 plots results of the number of iterations in various electric conductivity of the phantom. The electric conductivity from a saline to a metal were used. As can be seen, DDM-COCR and DDM-MINRES-like_CS got faster convergence rate, and especially DDM-MINRES-like_CS achieved an sigfinicant improvement of convergence rate at lower electric conductivity.

5. Conclusions

The COCG method is generally used to solve the high frequency electromagnetic problem. However, it suffers from oscillating convergence histories. To solve such large-scale complex symmetric systems, we have proposed the iterative substructuring based on the COCG method or the COCR method, but

Table 2: Computational performances in the case of $N = 640$ ($n_e/N \approx 170$) of TEAM29(small) model

	Number of iterations	Time (sec)	$log_{10} \frac{\|\boldsymbol{g}-\boldsymbol{S}\boldsymbol{u}_B^n\|}{\|\boldsymbol{g}-\boldsymbol{S}\boldsymbol{u}_B^0\|}$
DDM-COCG	2,884	75	-7.17
DDM-COCR	2,583	68	-7.16
DDM-QMR_SYM	2,606	69	-7.06
DDM-MINRES-like_CS	2,706	72	-7.05

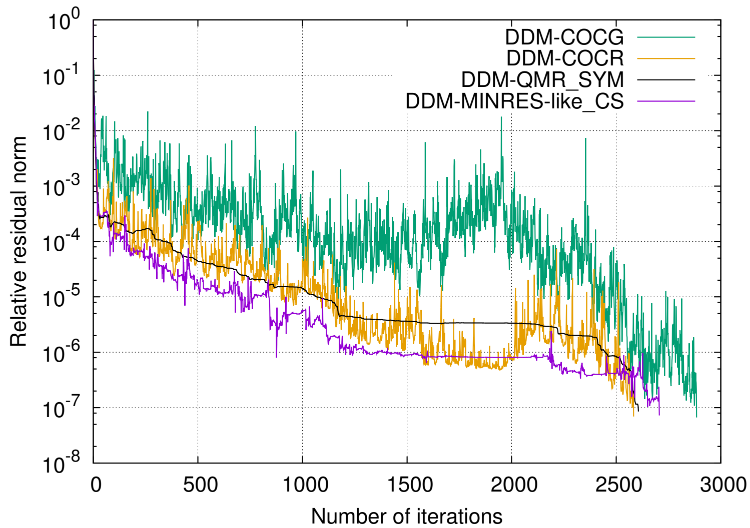

Figure 2: Convergence histories in the case of $N = 640$ ($n_e/N \approx 170$) of TEAM29(small) model

Table 3: Computational performances in the case of $N = 98,304$ ($n_e/N \approx 176$) of TEAM29(large) model

	Number of iterations	Time (sec)	$log_{10} \frac{\|\boldsymbol{g}-\boldsymbol{S}\boldsymbol{u}_B^n\|}{\|\boldsymbol{g}-\boldsymbol{S}\boldsymbol{u}_B^0\|}$
DDM-COCG	22,097	7,857	-7.04
DDM-COCR	10,236	3,751	-7.01
DDM-QMR_SYM	19,612	7,070	-7.00
DDM-MINRES-like_CS	6,214	2,329	-7.04

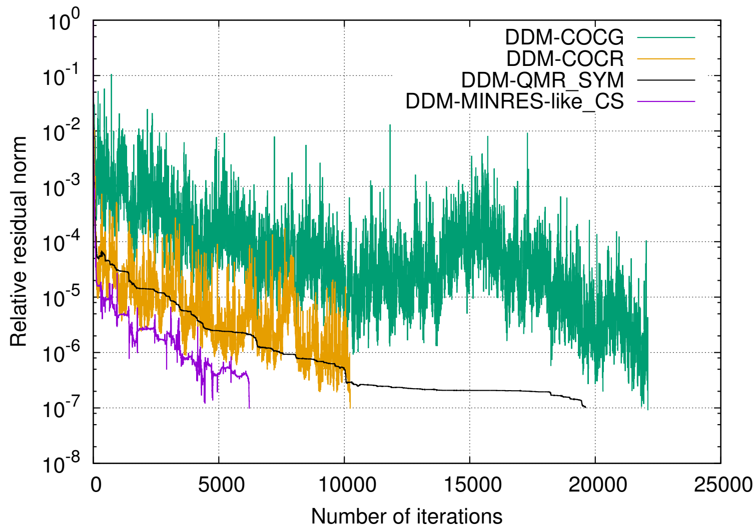

Figure 3: Convergence histories in the case of $N = 98,304$ ($n_e/N \approx 176$) of TEAM29(large) model

Table 4: Number of iterations with various number of subdomains in solving TEAM29(large) model

	n_e/N ≈ 88	n_e/N ≈ 176	n_e/N ≈ 352	n_e/N ≈ 704	n_e/N $\approx 1,408$	n_e/N $\approx 2,816$
DDM-COCG	25,100	22,097	18,105	15,164	14,783	13,322
DDM-COCR	14,937	10,236	10,720	9,480	9,065	7,932
DDM-QMR_SYM	23,633	19,612	16,948	13,516	12,326	11,409
DDM-MINRES-like_CS	7,035	6,214	5,448	5,819	6,632	5,550

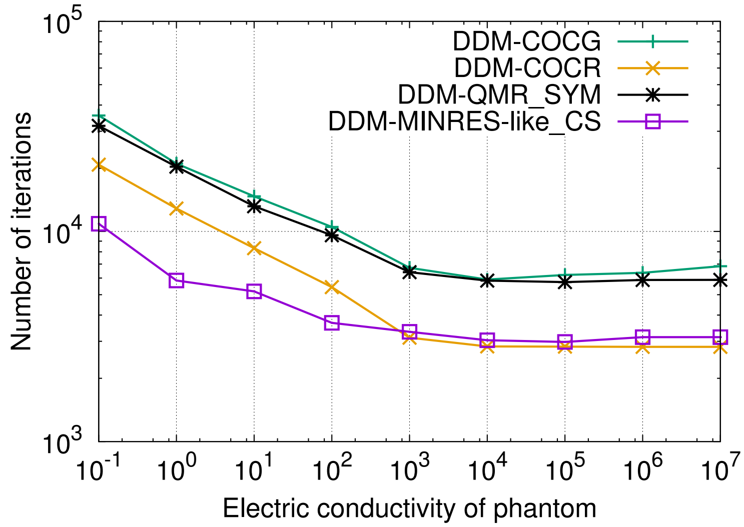

Figure 4: Electric conductivity of the dielectric phantom vs. the number of iterations in case of TEAM29(large) model

yet the issue remain unresolved. In this paper, as a variant MINRES method for complex symmetric systems, an MINRES-like_CS method is presented. Furthermore, an iterative substructuring method based on the method is also developed. The proposed method improved the convergence compared to other methods, and successfully reduced the computation time by about 70% compared to the COCG method in solving of a 20 million complex DOF case.

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