Preconditioning of Periodic Fast Multipole Method for Solving Volume Integral Equations

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***Abstract*—Application of FMM to the volume integral equations for periodic boundary value problem for Maxwell's equations is investigated. We propose effective preconditioners for the discretized volume integral equations. We confirm the accuracy and high performances of the proposed method in several numerical examples including periodic problems near Wood's anomalies.**

***Index Terms*—Fast multipole methods, Integral equations, Periodic structures, Preconditioner**

I. Introduction

Developing fast solvers for periodic boundary value problems is an important research subject because they are the basis of the analysis for periodic structures such as metamaterials and photonic crystals. Integral equation methods accelerated with FMM (Fast Multipole Method, [1]) are considered to be among promising candidates for such solvers. This is particularly true when the problem under consideration is of scattering type, since integral equation methods can deal with radiation conditions easily. In addition, we can take the effect of the periodicity into account in FMM using a few additional ingredients including lattice sums of the ordinary fundamental solution and its derivatives.

In this paper, we focus on doubly-periodic transmission problems for Maxwell's equations. An FMM-accelerated Boundary Integral Equation Method (BIEM) for such problems, called periodic FMM, has been proposed by Otani and Nishimura [2]. The periodic FMM uses the lattice sum expression of the periodic Green's function to regard a periodic boundary value problem as an ordinary problem with an infinite repetition of the replicas of the unit cell. Contributions from far replica cells can then be evaluated as the local expansion of the level 0 cell, and this expansion can be written with the lattice sums. The lattice sums depend only on the periods, wavenumber and the Floquet wavenumber and can be precomputed once for all in the FMM algorithm. Otherwise the algorithm is exactly the same as the ordinary FMM, which is a distinctive advantage of the periodic FMM.

In this paper, we consider a volume integral equation counterpart of the periodic FMM [2]. The volume integral equations are often used to analyze inhomogeneous media, as we can see in [3] and [4], to mention just a few. Fast solvers for VIEM have also been investigated e.g. in [5], where the discrete BCG-FFT algorithm for the computation of the scattered fields from three dimensional inhomogeneous dielectric scatterers has been presented. In [6], the Adaptive Integral Method (AIM) has been used to solve scattering problems for mixed dielectric and conducting objects with the help of volume-surface integral equations. In addition, acceleration of VIEM with FMM has been investigated in [7], [8] and [9]. Attempts to develop fast solvers for periodic structures using the VIEM or VSIE (Volume/Surface integral equation method) are found in [10], where the MultiLevel Green's Function Interpolation Method (MLGFIM) is used for the acceleration, and in [11], where the Accelerated Cartesian Expansion (ACE) method is used. However, applications of the periodic version of the genuine FMM to VIEM have not been investigated so far.

The most common approach in the FMM accelerated integral equation methods solves the discretized integral equations iteratively. It is crucial to reduce the number of iterations for solving linear equations in such approaches for the better computational efficiency. This is particularly the case in periodic problems because the convergence of the linear iterative solvers may deteriorate near Wood's anomalies, which are well-known phenomena in periodic problems where the solution of the problem varies dramatically for small changes of parameters [12]. In view of this, we discuss preconditioning issues in VIEM for periodic problems. We use the volume integral equations proposed by Schaubert et al. [13] to this end. We propose two preconditioners for discretized volume integral equations, which are usually considered well-conditioned but computationally intensive and do need preconditioners, as we shall see. We show that these preconditioners are effective in reducing the computational time of VIEM also near anomalies in periodic problems.

II. Formulation

A. Periodic boundary value problem

We consider doubly-periodic transmission problems for Maxwell's equations in 3D. We assume that the domain under consideration is periodic in the x_2 and x_3 directions, with the periods of L_2 and L_3, respectively. We define $\Omega_0 = (-\infty,\infty)\otimes[-L_2/2,L_2/2]\otimes[-L_3/2,L_3/2]$ to be the unit domain (i.e., the unit of periodicity) in which we have a finite scatterer Ω as shown in Fig.1. Our problem is to solve Maxwell's equations:

$$\nabla\times\boldsymbol{H}=-i\omega\epsilon\boldsymbol{E},\quad \nabla\times\boldsymbol{E}=i\omega\mu_0\boldsymbol{H} \tag{1}$$

for the electric field $\boldsymbol{E}$ and the magnetic field $\boldsymbol{H}$ subject to the following periodic boundary conditions:

$$\begin{aligned}\boldsymbol{E}(x_1,L_2/2,x_3)&=e^{i\beta_2}\boldsymbol{E}(x_1,-L_2/2,x_3)\\ \boldsymbol{E}(x_1,x_2,L_3/2)&=e^{i\beta_3}\boldsymbol{E}(x_1,x_2,-L_3/2)\\ \boldsymbol{H}(x_1,L_2/2,x_3)&=e^{i\beta_2}\boldsymbol{H}(x_1,-L_2/2,x_3)\\ \boldsymbol{H}(x_1,x_2,L_3/2)&=e^{i\beta_3}\boldsymbol{H}(x_1,x_2,-L_3/2),\end{aligned}$$

and the radiation condition for the scattered wave. Here, ω is the frequency (with the $e^{-i\omega t}$ time dependence), ϵ is the permittivity in Ω_0 and β_2 and $\beta_3\in\mathbb{R}$ are the (non-dimensional) Floquet wave numbers (phase differences of the

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incident wave) along x_2 and x_3 directions, respectively. In $\Omega_0 \setminus \overline{\Omega}$, where the wave number $k_e = \omega\sqrt{\epsilon_e \mu_0}$ is constant, we consider the incident plane wave of the following forms:

$$\boldsymbol{E}^0(\boldsymbol{x}) = \boldsymbol{a}^{\rm inc} e^{i\boldsymbol{k}^{\rm inc}\cdot\boldsymbol{x}},\ \boldsymbol{H}^0(\boldsymbol{x}) = \boldsymbol{b}^{\rm inc} e^{i\boldsymbol{k}^{\rm inc}\cdot\boldsymbol{x}}.$$

The Floquet wavenumber β_i is then expressed by $\beta_i = L_i k_i^{\rm inc}$. We assume that the permeability is equal to the vacuum permeability μ_0 everywhere and ϵ is a function of the position $\boldsymbol{x}$ given as follows:

$$\epsilon(\boldsymbol{x}) = \begin{cases} \epsilon(\boldsymbol{x}) & (\boldsymbol{x} \in \Omega) \\ \epsilon_e \text{ (const.)} & (\boldsymbol{x} \in \Omega_0 \setminus \overline{\Omega}). \end{cases}$$

We note that many periodic problems of interest, such as photonic crystals and metamaterials, belong to low frequency problems.

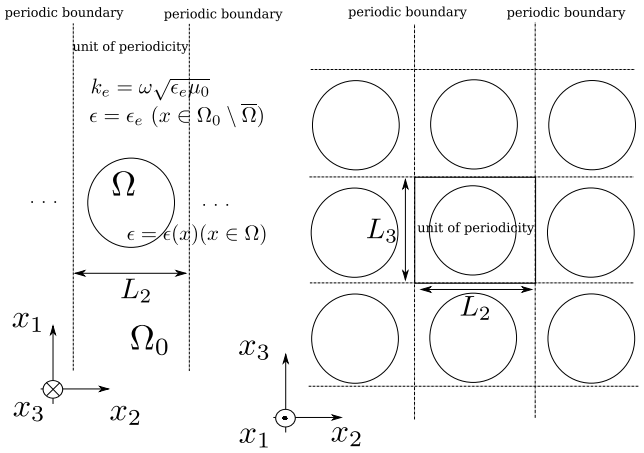


Fig. 1. Periodic boundary value problems. Ω_0 is the unit domain (unit of periodicity) which extends to $\pm\infty$ in x_1-axis, and Ω is a finite scatterer.

B. Volume integral equation

We consider the volume integral equation for the electric flux density $\boldsymbol{D}(\boldsymbol{x}) = \epsilon(\boldsymbol{x})\boldsymbol{E}(\boldsymbol{x})$ written as follows:

$$\frac{D_i(\boldsymbol{x})}{\epsilon(\boldsymbol{x})} - \omega^2\mu_0 \int_\Omega \Gamma_{ij}^P(\boldsymbol{x}-\boldsymbol{y})\kappa(\boldsymbol{y})D_j(\boldsymbol{y})d\boldsymbol{y} = E_i^0(\boldsymbol{x}) \quad (2)$$

where κ is a function given by $\kappa(\boldsymbol{x}) = (\epsilon(\boldsymbol{x}) - \epsilon_e)/\epsilon(\boldsymbol{x})$ and Γ_{ij}^P denotes the periodic Green's function which can be written as follows:

$$\Gamma_{ij}^P(\boldsymbol{x}-\boldsymbol{y}) = \left(\delta_{ij} + \frac{1}{k_e^2}\frac{\partial}{\partial y_i}\frac{\partial}{\partial y_j}\right) G^P(\boldsymbol{x}-\boldsymbol{y}) \quad (3)$$

$$G^P(\boldsymbol{x}-\boldsymbol{y}) = \sum_{\boldsymbol{\omega}\in\mathcal{L}} G(\boldsymbol{x}-\boldsymbol{y}-\boldsymbol{\omega})e^{i\boldsymbol{\beta}\cdot\boldsymbol{\omega}}$$

$$\mathcal{L} = \{\boldsymbol{\omega} = (0, n_2, n_3) | n_2, n_3 \in \mathbb{Z}\},\ \boldsymbol{\beta} = (0, \beta_2, \beta_3)$$

$$G(\boldsymbol{x}-\boldsymbol{y}) = \frac{e^{ik_e|\boldsymbol{x}-\boldsymbol{y}|}}{4\pi|\boldsymbol{x}-\boldsymbol{y}|} \quad (4)$$

and G and G^P are the fundamental solution and periodic Green's function of Helmholtz' equation, respectively. The second term on the LHS of (2) has a strong singularity at $\boldsymbol{x} \in \Omega$ which has to be interpreted in the sense of distribution. Written explicitly, the integral in (2) in $\boldsymbol{x} \in \Omega$ takes the following form:

$$\left(\frac{1}{\epsilon(\boldsymbol{x})} + \frac{\kappa(\boldsymbol{x})}{3\epsilon_e}\right) D_i(\boldsymbol{x}) - \omega^2\mu_0 \int_\Omega G^P(\boldsymbol{x}-\boldsymbol{y})\kappa(\boldsymbol{y})D_j(\boldsymbol{y})d\boldsymbol{y} - \frac{1}{\epsilon_e}\text{p.v.}\int_\Omega \frac{\partial}{\partial y_i}\frac{\partial}{\partial y_j} G^P(\boldsymbol{x}-\boldsymbol{y})\kappa(\boldsymbol{y})D_j(\boldsymbol{y})d\boldsymbol{y} = E_i^0(\boldsymbol{x}),\ \boldsymbol{x} \in \Omega \quad (5)$$

where p.v. stands for the standard Cauchy's principal value.

C. Discretization

Note that the unknown $\boldsymbol{D}$ in the integral equation in (2) is in $H_{\rm div}(\Omega)$. It is therefore reasonable to discretize (2) (or (5)) using the SWG (Schaubert-Wilton-Glisson) basis functions [13] for $\boldsymbol{D} \in H_{\rm div}(\Omega)$. We substitute this expansion into (2) and test it with the SWG basis function. Namely, we define $\boldsymbol{t}_m(\cdot)$ as the m-th SWG basis function and approximate $\boldsymbol{D}(\boldsymbol{x})$ by:

$$\boldsymbol{D}(\boldsymbol{x}) \approx \sum_n d_n \boldsymbol{t}_n(\boldsymbol{x}). \quad (6)$$

We thus obtain the following discretized version of the volume integral equation in (2):

$$\sum_n \left(\int_\Omega \frac{1}{\epsilon(\boldsymbol{x})} \boldsymbol{t}_m(\boldsymbol{x}) \cdot \boldsymbol{t}_n(\boldsymbol{x}) d\boldsymbol{x} - \int_\Omega \omega^2\mu_0 \boldsymbol{t}_m(\boldsymbol{x}) \cdot \int_\Omega \Gamma^P(\boldsymbol{x}-\boldsymbol{y}) \cdot \kappa(\boldsymbol{y})\boldsymbol{t}_n(\boldsymbol{y}) d\boldsymbol{y} d\boldsymbol{x} \right) d_n = \int_\Omega \boldsymbol{E}^0(\boldsymbol{x}) \cdot \boldsymbol{t}_m(\boldsymbol{x}) d\boldsymbol{x}. \quad (7)$$

The equation in (7) is solved for the coefficients d_n with the help of the periodic FMM [2] and a certain iterative solver.

D. Periodic FMM

FMM is a well-established fast algorithm to compute the matrix-vector product $A\boldsymbol{x}$ for the discretized integral equation. In this paper, we use the periodic version of the low-frequency FMM to evaluate the potential term in (2) given by:

$$V_i(\boldsymbol{x}) = -\omega^2\mu_0 \int_\Omega \left(\delta_{ij} + \frac{1}{k_e^2}\frac{\partial}{\partial y_i}\frac{\partial}{\partial y_j}\right) G^P(\boldsymbol{x}-\boldsymbol{y})\kappa(\boldsymbol{y})D_j(\boldsymbol{y})d\boldsymbol{y} \quad (8)$$

for $\boldsymbol{x} \notin \Omega$. As a matter of fact, the periodic FMM, developed for BIEM, can be used with VIEM with a minimal change of the definition of the multipole moments. We therefore show only the results, and do not elaborate on the periodic FMM here. See Otani and Nishimura [2] for further details.

The low-frequency FMM for non-periodic problem is based on the following expansion of G:

$$G(\boldsymbol{x}-\boldsymbol{y}) = \frac{ik_e}{4\pi}\sum_{n,m}(2n+1)I_n^m(\overrightarrow{\boldsymbol{x}_0\boldsymbol{x}}) \times \sum_{n',m'}(2n'+1)T_{n',n}^{m',m}(\overrightarrow{O\boldsymbol{x}_0})(-1)^{m'}I_{n'}^{-m'}(\overrightarrow{O\boldsymbol{y}}) \quad (9)$$

where O and $\boldsymbol{x}_0$ are points near $\boldsymbol{y}$ and $\boldsymbol{x}$, respectively, for which we assume that $|\overrightarrow{O\boldsymbol{x}_0}| > |\overrightarrow{\boldsymbol{x}_0\boldsymbol{x}} + \overrightarrow{O\boldsymbol{y}}|$ holds. The functions O_m^n and I_m^n are the radiating and entire solutions of Helmholtz' equation defined as follows:

$$O_n^m(\overrightarrow{O\boldsymbol{x}}) = h_n^{(1)}(k_e|\overrightarrow{O\boldsymbol{x}}|)Y_n^m\left(\frac{\overrightarrow{O\boldsymbol{x}}}{|\overrightarrow{O\boldsymbol{x}}|}\right)$$
$$I_n^m(\overrightarrow{O\boldsymbol{x}}) = j_n(k_e|\overrightarrow{O\boldsymbol{x}}|)Y_n^m\left(\frac{\overrightarrow{O\boldsymbol{x}}}{|\overrightarrow{O\boldsymbol{x}}|}\right)$$
$$Y_n^m\left(\frac{\overrightarrow{O\boldsymbol{x}}}{|\overrightarrow{O\boldsymbol{x}}|}\right) = \sqrt{\frac{(n-m)!}{(n+m)!}}P_n^m(\cos\theta)e^{im\phi}$$

where $h_n^{(1)}$ and j_n are the spherical Hankel function of the first kind and n-th order and the spherical Bessel function of the n-th order, (r,θ,ϕ) are the polar coordinates of the vector $\overrightarrow{O\boldsymbol{x}}$ and P_n^m is the associated Legendre function. The coefficients $T_{n',n}^{m',m}$ can be computed by a recurrence formula. Substituting (9) into the non-periodic version of (8), we obtain the following local expansion of the potential V_i:

$$V_i(\boldsymbol{x}) = \frac{i\omega\sqrt{\mu_0}}{4\pi\sqrt{\epsilon_e}}\sum_{n,m}(2n+1)L_{r,n}^m(\boldsymbol{x}_0)e_{iqr}\frac{\partial}{\partial x_q}I_n^m(\overrightarrow{\boldsymbol{x}_0\boldsymbol{x}}) \tag{10}$$

where $L_{i,n}^m(\boldsymbol{x}_0)$ is the coefficients of the local expansion around $\boldsymbol{x}_0$ which is defined by the following M2L formula:

$$L_{i,n}^m(\boldsymbol{x}_0) = \sum_{n',m'}(2n'+1)T_{n',n}^{m',m}(\overrightarrow{O\boldsymbol{x}_0})M_{i,n'}^{m'}(O) \tag{11}$$

and $M_{i,n}^m$ is the multipole moment around O:

$$M_{i,n}^m(O) = \int_\Omega e_{ipq}\frac{\partial}{\partial y_p}(-1)^m I_n^{-m}(\overrightarrow{O\boldsymbol{y}})\kappa(\boldsymbol{y})D_q(\boldsymbol{y})d\boldsymbol{y} \tag{12}$$

The shift formulae for $M_{i,n}^m$ and $L_{i,n}^m$ (M2M and L2L) are the same as those for the BIEM. In practice the infinite series in (10) and (11) are truncated. We use sufficient number of terms to assure 3 digits of accuracy in the examples to be shown later. The periodic FMM interprets periodic boundary value problems as ordinary boundary value problems for infinite replicas. The contributions from replicas near the unit cell are evaluated by the ordinary FMM and the effects from other replicas are computed using a periodic version of the M2L formula obtained by replacing $T_{n',n}^{m',m}(\overrightarrow{O\boldsymbol{x}_0})$ in (11) by the lattice sum given by:

$$\sum_{n_2,n_3}T_{n',n}^{m',m}(n_2L_2\boldsymbol{e}_2 + n_3L_3\boldsymbol{e}_3)e^{-i(n_2\beta_2+n_3\beta_3)} \tag{13}$$

where the summation is over indices for far replicas. See Otani and Nishimura [2] for a practical way of computing the sum in (13).

We note that the present formulation assumes that the structure is orthotropic. It is possible to extend the formulation to other cases, but the details remain to be worked out.

III. Preconditioners

In this section, we propose two preconditioners for (7).

It is generally believed that VIEMs produce well conditioned matrices. This is because the operator of the volume integral equation (2) is well-conditioned, as we can infer e.g. from the related spectral analysis in Costabel et al.[14] who noted that the essential spectrum of the integral operator in (2) (applied to κD_j and multiplied by ϵ_e, to be precise) consists of only 0, $1/2$ and 1 when Ω is homogeneous [14]. However, developing good preconditioners for VIEM is considered to be worth the efforts because reducing the already small number of iterations for VIEM even by a few times will have considerable effects on the overall computational time since VIEM tends to be computationally intensive.

A. Gram-Preconditioner

As the first preconditioner for (7) used with linear iterative solvers, we propose to use the first term of (7) as the right preconditioner:

$$P_{mn} = \int_\Omega \frac{1}{\epsilon(\boldsymbol{x})}\boldsymbol{t}_m(\boldsymbol{x})\cdot\boldsymbol{t}_n(\boldsymbol{x})d\boldsymbol{x}. \tag{14}$$

Obviously, this preconditioner is expected to work as a good scaling factor for (7) since the free term in (7) is reduced to an identity with this preconditioner. Another function of this preconditioner is to make the discretized system in (7) a better approximation to the original integral equation in (2) (See [15] for further explanation) in that the identity operator (multiplied by a scalar function, to be precise) is transformed into an identity matrix. As a matter of fact, the operator of the volume integral equation (2) is well-conditioned, as we have already noted. Therefore, we expect that the discretized equation in (7) will show better convergence with linear iterative solvers if the spectral properties of the discretized system is made closer to the original equation in (2).

We call this preconditioner as the Gram-preconditioner in this paper since the matrix defined by (14) is the Gram matrix. To implement the Gram-preconditioner in the iterative solver, the following steps are required for a candidate solution $\boldsymbol{y}$ at every iteration step in the iterative solver:

1) solve $P\boldsymbol{x} = \boldsymbol{y}$ for $\boldsymbol{x}$
2) compute the matrix-vector product $A\boldsymbol{x}$

Namely, the additional computational cost of the Gram-preconditioner is one inversion of P (i.e. solve $P\boldsymbol{x} = \boldsymbol{y}$) at every step of the iterative solver. P is a sparse matrix which can be easily inverted iteratively.

B. $AP^{-1}BQ^{-1}$-preconditioner

It can be shown that the operator defined by

$$(\mathcal{B}\phi)_j = \frac{\phi_j(\boldsymbol{x})}{\epsilon_e} + \omega^2\mu_0\int_\Omega \Gamma_{jk}^P(\boldsymbol{x}-\boldsymbol{y})\kappa(\boldsymbol{y})\phi_k(\boldsymbol{y})d\boldsymbol{y} \tag{15}$$

satisfies

$$\mathcal{A}\mathcal{B} = \frac{1}{\epsilon_e\epsilon(\boldsymbol{x})}(\mathcal{I}+\mathcal{K}) \tag{16}$$

when the domain Ω extends to infinity, where $\mathcal{A}$ is the operator on the LHS of (2) given by

$$(\mathcal{A}D)_i = \frac{D_i(\boldsymbol{x})}{\epsilon(\boldsymbol{x})} - \omega^2\mu_0 \int_\Omega \Gamma_{ij}^P(\boldsymbol{x}-\boldsymbol{y})\kappa(\boldsymbol{y})D_j(\boldsymbol{y})d\boldsymbol{y}, \quad (17)$$

$\mathcal{I}$ is the identity operator and $\mathcal{K}$ is a compact operator. To see this, we consider the homogeneous case (i.e., $\epsilon = \text{const.}$). The principal symbol of $\mathcal{A}$, or the Fourier transform of the most singular part of the kernel, is given as follows:

$$\frac{1}{\epsilon}\delta_{ij} + \left(\frac{1}{\epsilon_e} - \frac{1}{\epsilon}\right)\frac{\xi_i\xi_j}{|\boldsymbol{\xi}|^2} \quad (18)$$

where ξ_i is the Fourier variable. The inverse of (18), multiplied by $1/(\epsilon\epsilon_e)$, is given by:

$$\frac{1}{\epsilon_e}\delta_{jk} - \left(\frac{1}{\epsilon_e} - \frac{1}{\epsilon}\right)\frac{\xi_j\xi_k}{|\boldsymbol{\xi}|^2} \quad (19)$$

which is the principal symbol of $\mathcal{B}$, thus proving (16). The fact that (16) remains valid for the variable ϵ case may be shown with the help of the theory of pseudo differential operators (see [16] for example).

Using the same argument as has been used in III-A, we expect that the matrix given by

$$AP^{-1}BQ^{-1}$$

has a spectral property similar to that of $\mathcal{AB}$ and, hence, gives a well conditioned equation, where

$$Q_{mn} = \int_\Omega \frac{1}{\epsilon_e}\boldsymbol{t}_m(\boldsymbol{x})\cdot\boldsymbol{t}_n(\boldsymbol{x})d\boldsymbol{x},$$

and A and B are the discretized matrices for $\mathcal{A}$ and $\mathcal{B}$, respectively. We thus propose to right-precondition (7) using the matrix $QB^{-1}P$ as a preconditioner even when Ω is bounded. Note that the integral part of $\mathcal{B}$ is exactly the same as that for $\mathcal{A}$. In applying B, we can therefore make good use of the matrix-vector product implementation which we already have for A. In this paper, we call this preconditioner as the $AP^{-1}BQ^{-1}$-preconditioner. To implement the $AP^{-1}BQ^{-1}$-preconditioner, the following steps are required for a candidate solution $\boldsymbol{y}$ at every iteration step in the iterative solver:

1) solve $Q\boldsymbol{z} = \boldsymbol{y}$ for $\boldsymbol{z}$
2) compute the matrix-vector product $B\boldsymbol{z}$
3) solve $P\boldsymbol{x} = B\boldsymbol{z}$ for $\boldsymbol{x}$
4) compute the matrix-vector product $A\boldsymbol{x}$

The computational costs for steps 2 and 4 are almost identical and those for steps 1 and 3 are negligible. Hence this preconditioning is considered worth the efforts if it can reduce the number of iterations to less than $1/2$ of the original.

IV. Numerical examples

In this section, we test the proposed approaches with numerical examples. In all the examples shown below, we use an appropriate non-dimensionalization using ϵ_0 and μ_0 (the vacuum permittivity and permeability) and a certain unit of length l_0 [m]. With this non-dimensionalization, ϵ and μ are actually relative permittivity and permeability and we have $\epsilon_e = 1$ if the outer space is vacuum, which we assume in the following examples. Physical quantities are obtained as one multiplies the following quantities to the corresponding non-dimensional quantities: length: l_0, time: $\frac{l_0}{c_0}$, where $c_0 = 3.0\times 10^8$[m/s] is the speed of light. For example, the (dimensional) frequency f is given in terms of the non-dimensional circular frequency ω as $f = \frac{c_0\omega}{2\pi l_0}$[Hz]. As the linear iterative solver, we use FGMRES (Flexible Generalized Minimal RESidual Method) [17], which allows the use of iterative methods for the inversion of preconditioners. For the approximate inversion of the matrices P and Q in FGMRES, we use the ordinary GMRES. We set the tolerance (relative error) for both main FGMRES and for GMRES for the inversion of the matrix P and Q to be 10^{-5} and we set the maximum number of iterations of FGMRES to be 1000.

A. Comparison with exact solution — non-periodic case

To test the accuracy of the proposed method, we first consider a case in which we can obtain the exact solution. The scatterer is a single sphere (i.e. not periodic case) having the radius of 0.35, the permittivity ϵ in Ω is fixed to be $\epsilon = 4.0$, and the frequency is given by $\omega = \pi$ (i.e. the wavelength in vacuum is about $5.7\times$ radius of the scatterer). The incident wave is given as $\boldsymbol{E}^0(\boldsymbol{x}) = (e^{ik_e x_3}, 0, 0)$. We define the error as follows:

$$\text{relative error} = \sqrt{\frac{\int_\Omega |\boldsymbol{D}(\boldsymbol{x}) - \boldsymbol{D}_{\text{Mie}}(\boldsymbol{x})|^2 d\boldsymbol{x}}{\int_\Omega |\boldsymbol{D}_{\text{Mie}}(\boldsymbol{x})|^2 d\boldsymbol{x}}} \quad (20)$$

where $\boldsymbol{D}_{\text{Mie}}$ is the exact solution obtained by the the Mie series and $\boldsymbol{D}$ is the numerical solution obtained by our method. We discretize the sphere by 6091 tetrahedron (the number of unknowns is 12874). We found that the numerical solution agrees with the exact solution within 4.14% of relative error. The speedup of the total computational time obtained only by the FMM acceleration was 5.46 in this example.

To test our preconditioners in problems with higher contrast, we change ϵ in the scatterer to 24, and vary ω from 1.0 to 3.0 (i.e., the wavelength in the vacuum is from 17.9 to $5.98\times$ radius of the scatterer). We discretize the sphere with 135168 tetrahedrons (the number of unknowns is 276256). Fig.2(a) shows the total radar cross sections for this problem obtained by our method and the Mie-series. We see that the results of the proposed method are satisfactory even near the resonances at $\omega \approx 1.78$ and 2.58. Fig.2(b) shows the number of iterations in the FGMRES and Fig.2(c) shows the computational time (second) for the convergence of the FGMRES. The no-preconditioned method could not satisfy the error tolerance after 1000 iterations for $\omega > 1.2$. On the other hand, both Gram-preconditioned and $AP^{-1}BQ^{-1}$-preconditioned methods converged within 1000 iterations. This observation tells that preconditioning is necessary with VIEs which are believed to be well-conditioned and that our preconditioners are effective in high contrast problems.

B. Periodic spheres

We consider doubly-periodic spherical scatterers having radii of 0.35. The periods L_2 and L_3 are both 1.0. We discretize the sphere by 129160 tetrahedrons (the number of

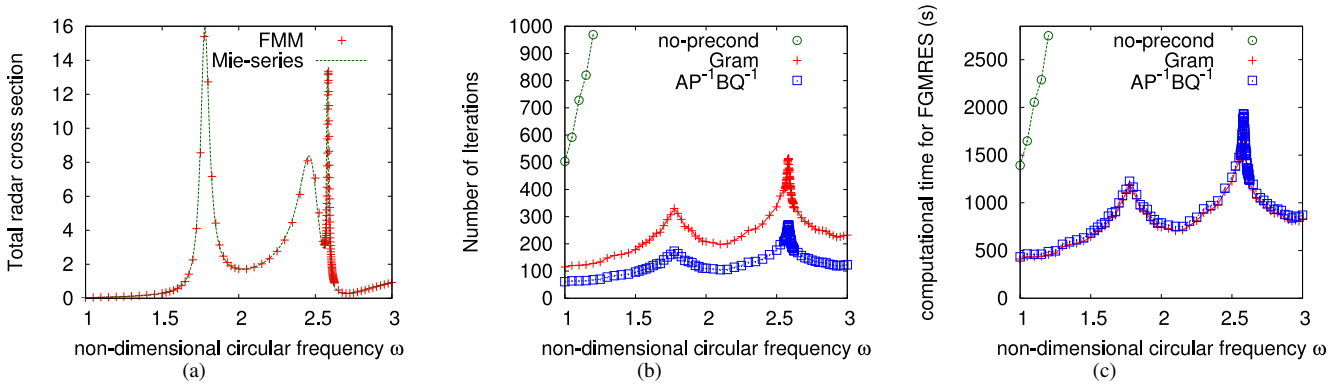


Fig. 2. non-periodic sphere, (a): Total radar cross section, (b): Number of iterations vs frequency, (c): Computational time(s) for FGMRES vs frequency

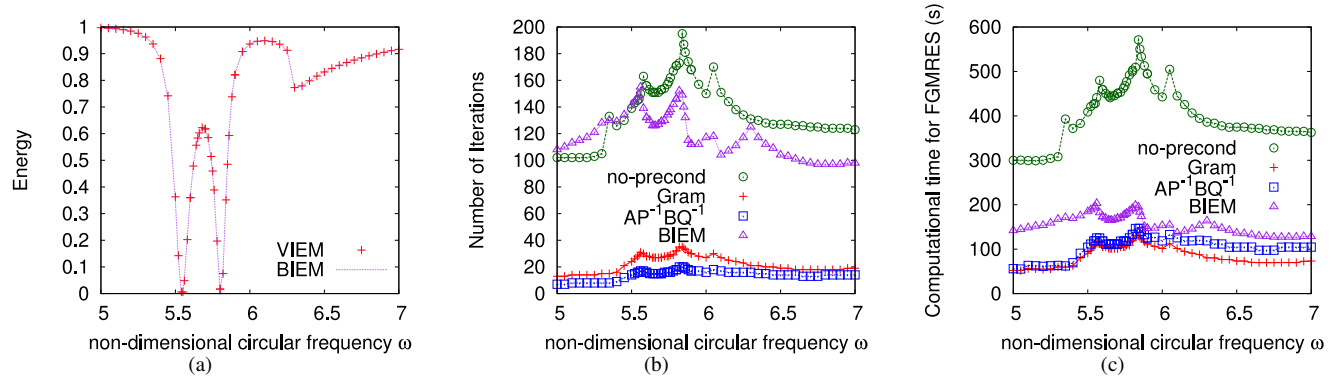


Fig. 3. periodic spherical scatterer, (a): Energy transmittance, (b): Number of iterations vs frequency, (c): Computational time(s) for FGMRES vs frequency

unknowns is 264039). Specifically, we test the performances of our method near Wood's anomalies.

The incident wave is given as follows ($\beta_3 = 0$):

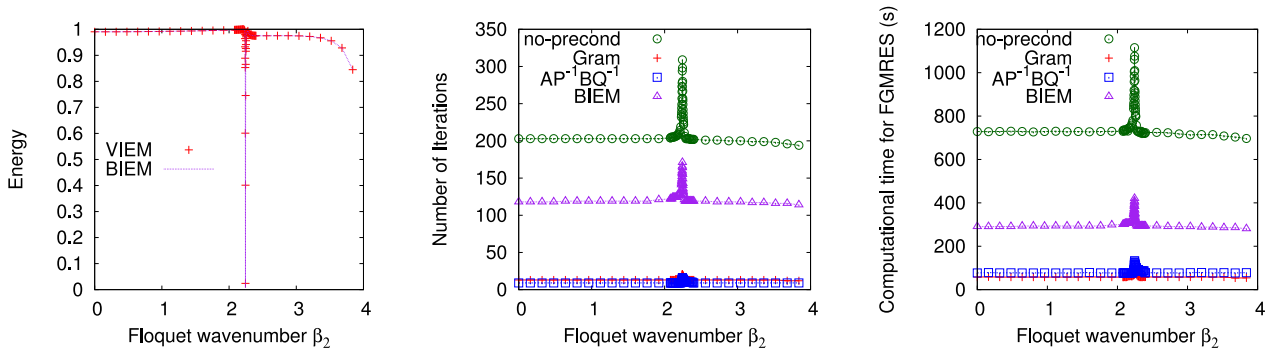
$$\boldsymbol{E}^0(\boldsymbol{x}) = \begin{pmatrix} \frac{\beta_2}{k_e L_2} \\ -\sqrt{1-\left(\frac{\beta_2}{k_e L_2}\right)^2} \\ 0 \end{pmatrix} e^{i\left(\sqrt{k_e^2-(\beta_2/L_2)^2}x_1+(\beta_2/L_2)x_2\right)}. \tag{21}$$

In this example, we set $\beta_2 = 0$ and fix $\epsilon = 2.56$ in the spheres. We vary ω from 5.0 to 7.0 (i.e., the wavelength in the vacuum varies from $1.26\times$ period to $0.90\times$ period, or $3.59\times$radius to $2.56\times$radius). We compare our results obtained with VIEM and those obtained with BIEM. In BIEM, we use the PMCHWT formulation and FGMRES as the linear iterative solver, with the part of the coefficient matrix representing the near field interaction as the right preconditioner [2]. As the tolerances for the main FGMRES and GMRES for the inversion of the near filed interaction coefficients matrix, we use 10^{-5} and 10^{-1}, respectively. In BIEM, we discretize the surface of the sphere into 11520 triangles (almost the same as the number of triangles on $\partial\Omega$ in the SWG mesh used for VIEM).

Fig.3(a) shows the energy transmittances computed with our method and those obtained with BIEM. These results agree well with each other. We also see that the computed energy transmittance approaches 0 at $\omega \approx 5.55$ and 5.8, thus indicating that these frequencies correspond to Wood's anomalies in this problem. We therefore test the performance of our method near $\omega \approx 5.55$ and 5.8.

Fig.3(b) shows the number of iterations in FGMRES. This figure shows that the numbers of iterations of the Gram-preconditioned method and the $AP^{-1}BQ^{-1}$-preconditioned method are much smaller than those of the no-preconditioned method. Besides, we see that the numbers of iterations for the Gram-preconditioned method and the $AP^{-1}BQ^{-1}$-preconditioned method do not increase very much even near Wood's anomalies. This is in contrast to the no-preconditioned method in which the number of iterations becomes large near Wood's anomalies. As a matter of fact, the numbers of iterations for the preconditioned VIEMs do increase near Wood's anomalies, but they remain under control thanks to the improved conditioning of the matrices obtained by the preconditioners.

Fig.3(c) shows the computational time in FGMRES. Note that the near-field interactions required in FMM are pre-computed and the corresponding computational time is excluded from the timing results. This figure shows the same tendency as the number of iteration. It is seen, however, that the Gram-preconditioned method is faster than the $AP^{-1}BQ^{-1}$-preconditioned method. This is because $AP^{-1}BQ^{-1}$-preconditioned method needs two matrix-vector products and two inversions of matrices P and Q in one iteration as discussed in III.



(a) (b) (c)

Fig. 4. periodic cubic scatterer, (a): Energy transmittance, (b): Number of iterations vs β_2, (c): Computational time(s) for FGMRES vs β_2

C. Periodic cubes

As an example of a non-smooth geometry, we consider cubic scatterers. Here, we consider a cube with a side length of $l = 0.35$, and discretize it into 163609 tetrahedrons (the number of unknowns is 338479). The incident wave is given by (21). We fix $\epsilon = 4$, $\omega = 4$ (i.e., the wavelength in the vacuum is $1.57\times$ period, the side length of the scatterer is $0.22\times$ the wavelength in vacuum) and vary β_2. Fig.4(a) shows the energy transmittances obtained with VIEM and BIEM (with 22118 triangles). The sharp dip near $\beta_2 \approx 2.24$ is considered to correspond to Wood's anomaly. Fig.4(b) and Fig.4(c) show the number of iterations and the computational time for FGMRES, respectively. We see that our preconditioners are effective also in this case, especially in the neighborhood of Wood's anomaly.

V. Conclusion

We summarize the results obtained in this paper as follows:

We extended the periodic FMM, which has been applied only to BIEM so far, to VIEM for doubly-periodic transmissions problems for Maxwell's equations. We then verified the proposed method in non-periodic problems by comparing the numerical solutions with the analytical results. The proposed method was then applied to periodic problems in which we found that the numerical solutions agreed with the BIEM solutions.

We also proposed two preconditioners. One is the Gram preconditioner in which we use the Gram matrix part of the discretized linear equation as the right preconditioner. The other is the $AP^{-1}BQ^{-1}$-preconditioner, which reduces the original integral operator essentially to a compact perturbation of an identity when the domain Ω is of infinite extent. This approach makes good use of matrices which we already have in the computation of the coefficient matrix for the original integral equation. With numerical examples, we verified that these preconditioners can reduce the number of iterations and the computational time for iterative solvers. We also found that our preconditioners work even in problems where no-preconditioned methods did not lead to convergence within reasonable numbers of iterations. In terms of the computational time, the Gram-preconditioned method is more efficient than the $AP^{-1}BQ^{-1}$-preconditioned method. These preconditioned methods remain effective even near Wood's anomalies where the non-preconditioned approach becomes inefficient.

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