Efficient Implementation of Inner-Outer Flexible GMRES for the Method of Moments Based on a Volume-Surface Integral Equation

Hidetoshi CHIBA†, Toru FUKASAWA†, Hiroaki MIYASHITA†, and Yoshihiko KONISHI†, Members

SUMMARY This paper presents flexible inner-outer Krylov subspace methods, which are implemented using the fast multipole method (FMM) for solving scattering problems with mixed dielectric and conducting objects. The flexible Krylov subspace methods refer to a class of methods that accept variable preconditioning. To obtain the maximum efficiency of the inner-outer methods, it is desirable to compute the inner iterations with the least possible effort. Hence, generally, inaccurate matrix-vector multiplication (MVM) is performed in the inner solver within a short computation time. This is realized by using a particular feature of the multipole techniques. The accuracy and computational cost of the FMM can be controlled by appropriately selecting the truncation number, which indicates the number of multipoles used to express far-field interactions. On the basis of the abovementioned fact, we construct a less-accurate but much cheaper version of the FMM by intentionally setting the truncation number to a sufficiently low value, and then use it for the computation of inaccurate MVM in the inner solver. However, there exists no definite rule for determining the suitable level of accuracy for the FMM within the inner solver. The main focus of this study is to clarify the relationship between the overall efficiency of the flexible inner-outer Krylov solver and the accuracy of the FMM within the inner solver. Numerical experiments reveal that there exists an optimal accuracy level for the FMM within the inner solver, and that a moderately accurate FMM operator serves as the optimal preconditioner.

key words: flexible GMRES, integral equation methods, method of moments, multilevel fast multipole algorithm, Krylov subspace methods

1. Introduction

Numerical methods for electromagnetic integral equations that describe scattering by or radiation from objects that are electrically large and complex have been intensely studied in recent years. This is due to the importance of research being conducted for many applications such as the prediction of the Radar Cross Section (RCS) of arbitrarily shaped three-dimensional (3D) objects and the design of antennas, etc. Among the various numerical methods, the method of moments (MoM) is one of the most powerful techniques; this method is generally implemented in conjunction with iterative linear system solvers. In recent times, Krylov subspace methods, which are used for iteratively solving linear systems, have enjoyed widespread success and popularity in scientific computing because of their wide range of applications. It is well known that the technique of using Krylov subspaces in iterative methods for solving linear systems is counted among the “Top 10” algorithms of the 20th century [1].

The lack of robustness is a widely recognized weakness of Krylov solvers. This is mainly the consequence of the fact that the convergence behavior of Krylov subspace methods strongly depends on the eigenvalue distribution of the coefficient matrix. The robustness can be improved by using preconditioning techniques. Preconditioning is simply the transformation of the original linear system into a system that yields the same solution, but is easier to solve with an iterative solver. However, since the FMM does not explicitly generate the coefficient matrix, establishing a strategy to design an efficient preconditioner for iterative methods implemented with the FMM continues to remain a challenging problem. The incomplete LU (ILU) and sparse approximate inverse (SAI) preconditioners, which are employed for the FMM implementation, were investigated in [2] and [3]. In both of these methods, the preconditioner is constructed from near-field interactions, which are readily available in the FMM algorithm. However, Malas [4] states that both of these methods become less effective when the problem size become very large. In recent years, novel iterative methods, which are classified as so-called flexible Krylov subspace methods, have been proposed [5],[6]. The flexible Krylov subspace methods refer to a class of methods that accept preconditioning that can change from one step to another. Malas [4] and Fan [7] have studied iterative solvers in the context of multipole techniques whose underlying fundamental concept is based on the flexible Krylov methods; the former study takes into account only the near-field interactions for the preconditioner, whereas the latter study includes the far-field interactions expressed by the multipole expansion as well as the near-field interactions for further enhancement of the preconditioner. However, thus far, iterative methods based on the flexible Krylov methods have been less extensively studied or practiced for electromagnetic wave problems. For the implementation of flexible Krylov inner-outer subspace methods, it is desirable to carry out the MVM within the inner solver with the least possible effort. However, no definite rule exists to determine the accuracy most suitable for the FMM within the inner solver. The main contribution of this paper is the clarification of the relationship between the overall efficiency of the flexible inner-outer Krylov solver and the accuracy of the MVM within the inner solver. In this study, we focus our attention, with regard to integral equation formulation, on the coupled volume-surface integral equation for solving scattering problems with mixed dielectric and conducting
objects. However, the strategies for the iterative methods described in this paper could be applied to other formulations. This paper is organized as follows. In Sect. 2, the coupled volume-surface integral equation formulation and the fundamentals of the FMM are outlined. A brief explanation of the flexible Krylov subspace method is provided in Sect. 3, and two parameters for controlling the accuracy and computational cost of the FMM within the inner solver are introduced. In Sect. 4, the efficiency of the flexible GMRES implemented with the proposed FMM operator for the inner solver is investigated. Finally, the conclusions are provided in Sect. 5.

2. Formulations

2.1 Volume-Surface Integral Equation

In this section, we formulate a coupled volume-surface integral equation for solving a scattering problem with mixed dielectric and conducting objects.

We consider an arbitrarily shaped three-dimensional (3D) scatterer that consists of an inhomogeneous dielectric material and perfectly electric conducting (PEC) body and resides in an isotropic homogeneous background medium of infinite extent, with \( \varepsilon_b \) and \( \mu_b \) representing the permittivity and permeability, respectively, as shown in Fig. 1. The dielectric region \( V \) is assumed to have position dependent permeability \( \mu(r_p) \) and permeability \( \mu_b \) in this paper. In addition, the \( e^{-i\omega t} \) time convention is assumed and suppressed, and the normalized vectors are indicated by \( \hat{\cdot} \) throughout this paper.

In the dielectric region \( V \), the total electric field is written as

\[
E(r_p) = E'(r_p) + E_V'(r_p) + E_S'(r_p),
\]

where \( E'(r_p) \) represents the incident wave and \( E_V'(r_p) \) and \( E_S'(r_p) \) indicate the scattered fields from the dielectric body and PEC body, respectively. On the PEC region \( S \), since the tangential components of the total electric field vanish, we have

\[
[E'(r_p) + E_V'(r_p) + E_S'(r_p)]_{\text{tan}} = 0.
\]

Using the equivalence principle, the dielectric body is removed and replaced by volume electric polarization currents \( J_V \) distributed in \( V \), and the surface of the PEC region \( S \) is replaced by surface electric currents \( J_S \). The scattered fields \( E_{\Omega}^s(r_p) \) and \( E_\Omega^b(r_p) \) produced by the induced volume and surface currents are given as follows:

\[
E_{\Omega}^s(r_p) = \int_{\Omega} G(r_p, r_q) \cdot J_{\Omega}(r_q) d\Omega, \quad \Omega = V \text{ or } S \tag{3}
\]

with

\[
\hat{G}(r_p, r_q) = -i\omega \mu_b \left( \hat{I} - \frac{1}{k_b^2} \nabla \nabla' \right) g(r_p, r_q), \tag{4}
\]

\[
g(r_p, r_q) = \frac{e^{ik_b|r_p - r_q|}}{4\pi |r_p - r_q|}, \tag{5}
\]

where \( k_b \) represents the wavenumber of the background material.

Now, defining a linear operator \( \tilde{L}_\Omega \) as

\[
\tilde{L}_\Omega(r_p, r_q) J_{\Omega}(r_q) = \int_{\Omega} \hat{G}(r_p, r_q) \cdot J_{\Omega}(r_q) d\Omega, \quad \Omega = V \text{ or } S, \tag{6}
\]

Eqs. (1) and (2) are rewritten in the following forms, respectively [8]:

\[
E(r_p) - \tilde{L}_V(r_p, r_q) J_V(r_q) - \tilde{L}_S(r_p, r_q) J_S(r_q) = E'(r_p), \quad r_p \in V, \tag{7}
\]

\[
-\left[ \tilde{L}_V(r_p, r_q) J_V(r_q) + \tilde{L}_S(r_p, r_q) J_S(r_q) \right]_{\text{tan}} = \left[ E'(r_p) \right]_{\text{tan}}, \quad r_p \in S. \tag{8}
\]

We notice that the total electric field on the left-hand side of Eq. (7) is related to the volume current by

\[
J_V = -i\omega [\varepsilon - \varepsilon_b] E. \tag{9}
\]

2.2 Method of Moments and Fast Multipole Method

To solve the volume integral Eqs. (7) and (8), the MoM is applied to discretize the equations into a matrix system. To this end, we employ the Rao-Whiton-Glisson (RWG) basis function [9], [10] so that regions \( V \) and \( S \) are discretized into a number of tetrahedral and triangular meshes, respectively. The surface current on \( S \) is expanded as

\[
J_S = \sum_{q=1}^{N_s} x_q^S j_q^S(r_q). \tag{10}
\]

As for the dielectric region \( V \), the electric flux \( D \) is expanded as follows:

\[
D = \varepsilon(r_q) E = \frac{1}{\iota \omega \varepsilon(r_q)} \sum_{q=1}^{N_s} x_q^V f_q^V(r_q). \tag{11}
\]

Using Eq. (9), the induced volume current is expressed as

\[
J_V = -i\omega \left[ \varepsilon(r_q) - \varepsilon_b \right] \frac{1}{\iota \omega \varepsilon(r_q)} \sum_{q=1}^{N_s} x_q^V f_q^V(r_q).
\]
where the right-hand side of Eq. (13) can be computed by
\[
\begin{bmatrix}
Z^V & Z^S \\
Z^S & Z^S
\end{bmatrix}
\begin{bmatrix}
I^V \\
I^S
\end{bmatrix} = \begin{bmatrix}
E^V \\
E^S
\end{bmatrix},
\]
(13)
where \( I^V \) and \( I^S \) are the unknown coefficients of the volume and surface current, respectively. The excitation vector on the right-hand side of Eq. (13) can be computed by
\[
E^\Omega_p = \int_\Omega f_p^\Omega(r_p) \cdot E'(r_p) d\Omega, \quad \Omega = V \text{ or } S.
\]
(14)
The elements of the block matrices are obtained as
\[
\tilde{Z}^{\Omega,\Omega} = \Delta^{\Omega,\Omega} + \bar{L}^{\Omega,\Omega},
\]
where
\[
\Delta^{\Omega,\Omega} = \left\{ \begin{array}{ll}
\int_{\Omega_p} f_p^\Omega(r_p) \cdot f_p^{\Omega^*(r_p)} d\Omega_p \\
0
\end{array} \right.
\]
if \( p = q \) and \( \Omega_p = \Omega_q = V \),
\[
L^{\Omega,\Omega} = -i\omega\mu_t \int_{\Omega_p} f_p^{\Omega}(r_p) \cdot \bar{G}(r_p, r_q) \cdot \chi'(r_q) f_q^{\Omega^*(r_q)} d\Omega_q d\Omega_p,
\]
(15)
\[
\chi'(r_q) = \begin{cases} 
\chi(r_q) & \text{if } \Omega_q = V \\
1 & \text{if } \Omega_q = S.
\end{cases}
\]
(16)
Finally, we summarize the formulation based on the fast multipole method. The MoM matrix elements corresponding to the far-field interactions of Eq. (17) can be expressed as follows [8]:
\[
L^{\Omega,\Omega} = -i\omega\mu_t \int d^2 k F_{pl}(\hat{k}) \cdot T_L(k, r_{LM}) F_{Mq}(\hat{k}),
\]
(17)
where
\[
F_{pl}(\hat{k}) = \int_{\Omega_p} dr_p e^{i k \cdot r_p} (I - \hat{k} \cdot \hat{k}) \cdot f_p^{\Omega^*(r_p)} d\Omega_p
\]
(18)
\[
F_{Mq}(\hat{k}) = \int_{\Omega_q} dr_q e^{i k \cdot r_q} (I - \hat{k} \cdot \hat{k}) \cdot \chi'(r_q) f_q^{\Omega^*(r_q)} d\Omega_q.
\]
(19)
and,
\[
T_L(k, r_{LM}) = \frac{ik}{16\pi^2} \sum_{l=0}^L (l+1) J_l^{(1)}(k r_{LM}) P_l(\hat{k} \cdot \hat{r}_{LM})
\]
(20)
in which \( h_l^{(1)}(\cdot) \), the spherical Hankel function of the first kind and of order \( l \); \( P_l(\cdot) \), the Legendre polynomial of order \( l \). The vector definitions are illustrated in Fig. 2.

Various methods have been developed for selecting the truncation number \( L \). A refined formula is provided in [11]:
\[
L = kd + 1.8d_0^{2/3}(kd)^{1/3},
\]
(21)
where \( d_0 \) denotes the desired correct number of digits, and it is set to 3 throughout this paper.

### 3. Inner-Outer Flexible GMRES

The flexible Krylov subspace methods belong to a class of methods that allow variable preconditioning; in other words, these methods accept preconditioning that can vary at each iteration step. Assume that the following system is solved:
\[
Ax = b,
\]
where \( A \) denotes the coefficient matrix, and \( x \) and \( b \) are vectors. In the conventional preconditioned Krylov solvers, the right-hand preconditioning operation \( z = K^{-1}v \) must be calculated in each iteration, where \( z \) and \( v \) are vectors and \( K \) is the preconditioning matrix. The preconditioner \( K \) must be a good approximation to \( A \), and it must be relatively cheap to construct. The operation \( z = K^{-1}v \) can be considered to be a method for approximately solving \( Az = v \). Hence, we can replace the computation of \( z = K^{-1}v \) by an alternative method, that is, we roughly solve the system \( Az = v \) by an iterative solver to obtain \( z \) instead of calculating \( z = K^{-1}v \). Here, the iterative solver for the original linear system is generally referred to as the “outer” solver, and the iterative solver that performs the preconditioning is referred to as the “inner” solver. This inner-outer concept implies that different values of \( K \) are obtained at each step of the Krylov method; hence, the outer solver must be able to work with variable preconditioners. This is facilitated by the use of flexible Krylov methods. It should be noted that a specific residual error within the inner solver does not affect the accuracy of the solution of the original linear system because the result of the inner solver is only used for the preconditioning. In addition, we also note that the particular case where the flexible GMRES (FGMRES) is employed for the outer solver and the GMRES is used for the inner solver is usually called “inner-outer flexible GMRES.”

To obtain maximum efficiency of the inner-outer methods, it is desirable to compute the inner iterations with the least possible effort. Hence, in general, inaccurate MVM
is performed in the inner solver within a short computation time. This is realized by using a particular feature of the multipole techniques. The accuracy and computational cost of the FMM can be controlled by selecting the truncation number, which indicates the number of multipoles used to express far-field interactions. On the basis of this fact, we construct a less-accurate but much cheaper version of FMM by intentionally setting the truncation number to a sufficiently lower value, and then use it for inaccurate MVM computation in the inner solver. We construct two FMM operators with different levels of accuracy. One of these operators is highly accurate and was used for the MVM within the outer solver, whereas the other operator, which is less accurate and a cheaper version of FMM, is used for the computation of the MVM within the inner solver.

To control the accuracy and computational cost of the FMM operator, we introduce two parameters, $L_{\text{low}}$ and $p$. $L_{\text{low}}$ defines the truncation number for the lowest MLFMA level within the inner solver. This parameter should be carefully treated in order to maintain its computational cost. In the FMM operation, the overall CPU time is mainly associated with the computation of the radiation pattern of the basis functions ($q2M$ translation or $q2M$) and the receiving pattern of the testing functions ($L2p$ translation or $L2p$) at the lowest MLFMA level. Correspondingly, $k$-space quadrature samples over the Ewald sphere of the basis functions ($q2M$ translator) and testing functions ($L2p$ translator) constitute a large portion of the overall memory requirements, and also directly depend on the truncation number for the lowest MLFMA level. Therefore, $L_{\text{low}}$ plays a key role in defining the computational cost of the FMM within the inner solver. The parameter $p$ defines the increasing rate of the truncation number when the level increases from the lowest to the highest, and it indicates the overall accuracy and computational cost. By using these two parameters, we can define the truncation number for the FMM within the inner solver, $L_i$, as follows:

$$L_i = c(ka)^p,$$

(23)

where $a$ denotes the cluster size of a level, and $c$ is a constant that is pre-computed prior to the solver execution according to the value of $L_{\text{low}}$, that is, $c$ is set such that $L_i$ for the lowest MLFMA level becomes equal to $L_{\text{low}}$. We notice that for the determination of the two parameters $L_{\text{low}}$ and $p$, both parameters should be set such that all the truncation numbers for the inner iteration ($L_i$) are less than those for the outer iteration ($L$). From Eq. (23), it is inferred that $p$ affects the overall accuracy and computational cost; as $p$ increases, the FMM within the inner solver becomes more accurate and increasingly more expensive.

4. Numerical Experiments

In this section, some numerical results will be presented to verify the efficiency of the inner-outer flexible GMRES with the proposed inner solver implemented in the multipole context.

We consider the following three geometries in the numerical experiments (see Fig. 3):

(a) Dielectric-coated conducting sphere,

(b) Dielectric-coated conducting NASA almond,

(c) Frequency selective surface (FSS) structure.

The first geometry (a) is a dielectric-coated conducting sphere. Since the analytical solution (Mie series) is available for this test case, it provides a reference solution for evaluating the accuracy of our software. The core of the conducting sphere has a radius of $5\lambda$, and the thickness of the dielectric layer, having a relative permittivity $\varepsilon_r = 1.5 - i0.5$, is $0.25\lambda$. The volume of the dielectric layer and the surface of the PEC sphere are discretized into $338,074$ tetrahedrons and $53,432$ triangular patches, respectively, leading to a total of $812,114$ unknowns. In this test case, the solver generates four MLFMA levels with the truncation number for the outer solver’s FMM being $[10, 15, 24, 41]$. Next, a dielectric-coated NASA almond is considered as the second test case (b). The dimensions of the PEC body are $32.02\lambda \times 12.35\lambda \times 4.20\lambda$, and the dielectric layer has a thickness of $0.1\lambda$, with a relative permittivity $\varepsilon_r = 1.5 - i0.5$. $93,042$ tetrahedrons and $38,208$ triangles are generated for the volume and surface region, respectively, resulting in a total of $274,463$ unknowns. For this example, the MLFMA operator in the outer solver consists of five levels, and $[9, 13, 20, 33, 58]$ are used as the truncation numbers. The
third test example (c) deals with an FSS structure that is \(10.1 \times 10.1 \times 0.1\lambda\), which is discretized into 60,796 tetrahedrons and 206,400 triangles, where the degrees of freedom for the resultant linear system become 424,504. The relative permittivity of the dielectric layer is \(\varepsilon_r = 1.1\). This test case yields four levels MLFMA operator within the outer solver, with the truncation number being \(10, 14, 23, 39\). This last example is the most realistic and complicated problem and is the most difficult to solve among the three geometries. In all of the cases, the scatterers are illuminated by an x-polarized and \(-z\)-traveling incident plane wave.

For the aforementioned three test cases, we conduct comparative experiments with respect to various sets of \(L_{\text{low}}\) and \(p\) introduced in the previous section. In addition, for comparison purpose, the strategies for the FMM operator within the inner solver employed in Malas [4] and Fan [7] as well as non-preconditioned GMRES case will also be investigated. Hereafter, we refer to the strategy proposed in [4] as “Malas’ strategy,” and that adopted in [7] as “Fan’s strategy.” The settings and conditions for the inner-outer flexible GMRES for all the strategies are summarized in Table 1. The same settings are used for all the three test cases. As shown in Table 1, we use two stopping criteria for both of the inner and outer solver; one of the criteria is error-bound (tolerance) and the other is the maximum number iterations. The settings for the Maras’ and Fan’s strategies shown in Table 1 are consistent with those in their original studies of [4] and [7].

It should be pointed out that Malas’ strategy has a noticeable feature in that the truncation number for FMM within the inner solver is equivalent to that for the FMM within the outer solver, and Fan’s strategy does not take into account the far-field interaction expressed by the multipole expansion within the outer solver. It should be also noted that the comparison among all the strategies is fair with regard to memory requirements. In fact, for the same restart value, the storage requirements for FGMRES are twice that for the standard GMRES, because FGMRES also stores the preconditioned vectors of the Krylov basis as well as the original Krylov basis. Further, for the inner solver, we do not restart and perform a prescribed number of full GMRES iterations. All the runs have been performed in single precision on one processor of a SGI Altix450 server with Itanium 2 processor.

Fig. 4 displays the bistatic RCS for the dielectric-
Table 2  Comparison of CPU time for presented strategy with various sets of $L_{lw}$ and $p$, along with Malas’ strategy [4], Fan’s strategy [7], and non-preconditioned GMRES(100); Acronyms: N.C. ≡ “not converged.”

(a) Dielectric-coated conducting sphere

<table>
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<tr>
<th>$L_{lw}$</th>
<th>$p$</th>
<th>$L_{l}$</th>
<th>Iteration times</th>
<th>CPU time [s]</th>
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(b) Dielectric-coated NASA almond

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(c) FSS structure

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<td>0.1</td>
<td>9, 9, 10, 11, 11</td>
<td>N.C.</td>
<td>N.C.</td>
<td></td>
</tr>
<tr>
<td>10</td>
<td>0.4</td>
<td>9, 11, 15, 20, 27</td>
<td>110</td>
<td>94949.59</td>
</tr>
<tr>
<td>0.58</td>
<td>9, 13, 20, 30</td>
<td>107</td>
<td>99498.96</td>
<td></td>
</tr>
<tr>
<td>Malas’ [4]</td>
<td>10, 11, 12, 16</td>
<td>N.C.</td>
<td>N.C.</td>
<td></td>
</tr>
<tr>
<td>Fan’s [7]</td>
<td>0, 0, 0, 0</td>
<td>N.C.</td>
<td>N.C.</td>
<td></td>
</tr>
<tr>
<td>Non-preconditioned GMRES(100)</td>
<td>N.C.</td>
<td>N.C.</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

coded conducting sphere of test case (a), calculated by the inner-outter flexible GMRES and Mie series. It can be observed that inner-outter flexible GMRES agrees quite well with the Mie series for both polarizations, validating the accuracy of the solver code that we developed.

Table 2 tabulates the iteration times and the CPU time required for the convergence for the presented strategy with various sets of $L_{lw}$ and $p$, along with Malas’ strategy [4], Fan’s strategy [7], and non-preconditioned GMRES(100), and Fig.5 compares the convergence history for the presented strategy with $(L_{lw}, p) = (6, 0.75)$, Malas’ strategy [4], Fan’s strategy [7], and non-preconditioned GMRES(100). From Table 2, it can be inferred that the combination $(L_{lw}, p) = (6, 0.75)$ perform quite well among all of the sets for all three test cases. Especially, it is worth noticing that, in the test case (c), the proposed method is the one that attains the solution, and all the other methods fail to converge. This observation reveals that there is an optimal
From the observations provided, we can state that the proposed strategy with \((L_{\text{low}}, p) = (6, 0.75)\) achieves the optimal performance with regard to the balance between the memory requirements and convergence behavior.

5. Conclusions

In this paper, we have reported the performance of the inner-outer flexible GMRES, implemented in the context of FMM techniques. Specifically, we have investigated the relationship between the overall performance of the inner-outer flexible GMRES and the accuracy of the MVM within the inner solver. We introduced two parameters for controlling the accuracy and computational cost of the inner FMM operator with the solver. In the numerical experiments, we employed the volume-surface integral equation for solving scattering problems with mixed dielectric and conducting objects. These numerical experiments revealed that there is an optimal accuracy for the FMM within the inner solver, and that a moderately accurate FMM operator serves as an optimal preconditioner. By using the preconditioner with the optimal accuracy, even though we require a slightly larger amount of memory storage compared to conventional methods, the proposed method significantly enhanced the convergence behavior.

References


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