[共同研究成果]

Convergence Property of Flexible GMRES for the Method of Moments Based on a Volume-Surface Integral Equation

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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 object. 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. To this end, 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 matrix-vector multiplication in 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 exits an optimal accuracy level for the FMM within the inner solver, and that a moderately accurate FMM operator serves as the optimal preconditioner. The accomplishments presented in this paper would contribute to not only the facilitation of the utilization of numerical methods for electromagnetic wave problems but also the further development of the computer aided engineering (CAE) technology.

1. Introduction

Amongst various numerical methods, the method of moments (MoM) is one of the most powerful techniques for solving large-scale electromagnetic wave problems, and it is usually implemented in conjunction with iterative linear system solvers. Recently, in the area of scientific computations, Krylov subspace methods (KSM), which are used for iteratively solving linear systems, have enjoyed widespread success and popularity in scientific computing because of significant advantages such as low memory requirements and good approximation properties.

Since the fast multipole method (FMM) [1] does not explicitly generate the coefficient matrix, it has been still a challenging problem to establish a strategy to design an efficient preconditioner for iterative methods implemented with the FMM. In recent years, novel iterative methods, which are classified as so-called flexible KSM, have been proposed [2][3]. The flexible KSM refer to a class of methods which accept preconditioning that can change from one step to the next. Malas [4] and Fan [5] have studied the flexible KSM in the context of multipole techniques; the former takes into account only the near field interaction for the preconditioner, whereas the latter includes also the far field interaction expressed by the multipole expansion as well as the near field interaction for further enhancement of the preconditioner. However, the flexible KSM have been less extensively studied or practiced so far for the electromagnetic wave problems. In this paper,

we propose an efficient implementation of the inner-outer flexible GMRES (FGMRES) in the context of the multipole techniques. The main contribution of this paper is to clarify the relation between overall efficiency of the inner-outer FGMRES and the accuracy of the inner solver's matrix-vector multiplication (MATVEC).

2. 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 system $\boldsymbol{Ax}=\boldsymbol{b}$ is solved, where $\boldsymbol{A}$ denotes the coefficient matrix, $\boldsymbol{b}$ is the right hand side vector, and $\boldsymbol{x}$ represents the unknown vector. In the conventional right-hand preconditioned algorithm, the right-hand preconditioning operation $\boldsymbol{z}=\boldsymbol{K}^{-1}\boldsymbol{v}$ is calculated in each iteration, where $\boldsymbol{z}$ and $\boldsymbol{v}$ are vectors and $\boldsymbol{K}$ is the preconditioning matrix. The preconditioner $\boldsymbol{K}$ must be a good approximation to $\boldsymbol{A}$, and it should be relatively cheap to construct. Here, the operation $\boldsymbol{z}=\boldsymbol{K}^{-1}\boldsymbol{v}$ can be considered to be a method for approximately solving $\boldsymbol{Az}=\boldsymbol{v}$. Hence, we can replace the computation $\boldsymbol{z}=\boldsymbol{K}^{-1}\boldsymbol{v}$ by roughly solving $\boldsymbol{Az}=\boldsymbol{v}$ with an iterative solver to obtain $\boldsymbol{z}$. 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 $\boldsymbol{K}$ are obtained at each step of the KSM; hence, the outer solver must be able to work with variable preconditioners. This is facilitated by the use of flexible KSM. 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 MATVEC 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 MATVEC computation in the inner solver. Accordingly, two FMM operators with different levels of accuracy are used; the one is highly accurate and was used for the MATVEC within the outer solver, whereas the other operator, which is less accurate and a cheaper version of FMM, is employed for the computation of the MATVEC within the inner solver.

To control the accuracy and computational cost of the FMM operator, we introduce two parameters, L_{low} and p. L_{low} defines the truncation number for the lowest MLFMA level 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:

$$L_i = c(ka)^p, \qquad (1)$$

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_{low}, that is, c is set such that L_i for the lowest MLFMA level becomes equal to L_{low}. We notice that for the determination of the two parameters L_{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. From Eq. (1), 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.

3. 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:

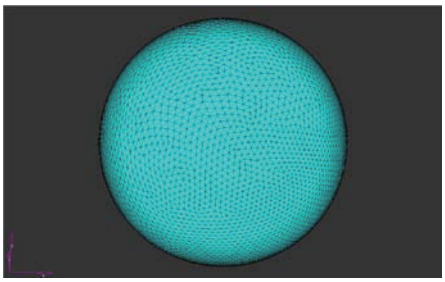
(a) Dielectric-coated conducting sphere,

(b) Dielectric-coated conducting NASA almond,

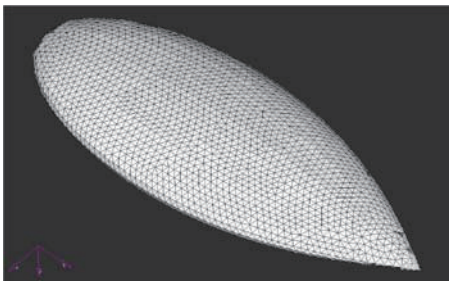
(c) Frequency selective surface (FSS) structure.

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 5λ, and the thickness of the dielectric layer, having a relative permittivity $\varepsilon_r = 1.5 - i0.5$, is 0.25λ. 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 0.1λ, 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 $10\lambda \times 10\lambda \times 0.1\lambda$, 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 $\{10,14,23,39\}$. All the truncation numbers are defined using the equation shown in [7]. 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.

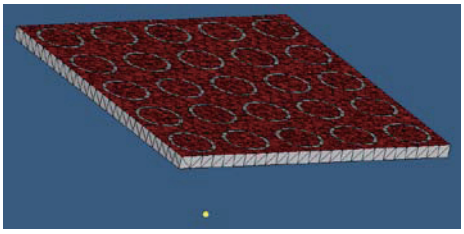
For the aforementioned three test cases, we conduct comparative experiments with respect to various sets of L_{low} and p introduced in the previous section. In addition, for comparison purpose, the strategies for the FMM operator within the inner solver employed in Malas [4] and Fan [5] as well as non-preconditioned GMRES case will also be investigated. Hereafter, we refer to the strategy proposed in [4] as "Malas' strategy," and that adopted in [5] 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 [5].



(a) Dielectric-coated conducting sphere



(b) Dielectric-coated conducting NASA almond



(c) FSS structure

Fig. 1 Geometry of three test examples.

Table 1: Settings and conditions for inner-outer flexible GMRES.

(a) Proposed strategy

Inner GMRES	Maximum number of iterations	20
	Tolerance	0.1
	Definition of the truncation number	Eq. (23)
	Restart cycle	20
Outer FGMRES	Maximum number of iterations	1000
	Tolerance	1.0E-4
	Restart cycle	40

(b) Malas' strategy [4]

Inner GMRES	Maximum number of iterations	10
	Tolerance	0.1
	Definition of the truncation number	Eq. (2) in [4]
	Restart cycle	10
Outer FGMRES	Maximum number of iterations	1000
	Tolerance	1.0E-4
	Restart cycle	45

(c) Fan's strategy [5]

Inner GMRES	Maximum number of iterations	7
	Tolerance	0.1
	Definition of the truncation number	-
	Restart cycle	7
Outer FGMRES	Maximum number of iterations	1000
	Tolerance	1.0E-4
	Restart cycle	47

(d) Non-preconditioned GMRES

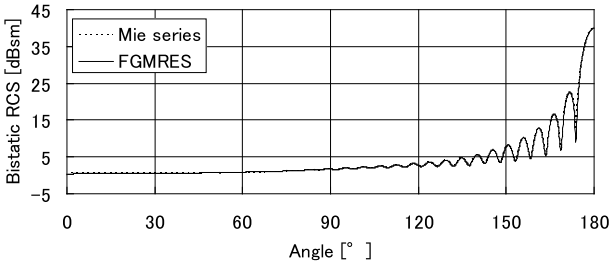
Inner GMRES	Maximum number of iterations	-
	Tolerance	-
	Definition of the truncation number	-
	Restart cycle	-
Outer FGMRES	Maximum number of iterations	2000
	Tolerance	1.0E-4
	Restart cycle	100

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 inner 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 a parallel computer Express5800 of Cyberscience Center, Tohoku University, Japan.

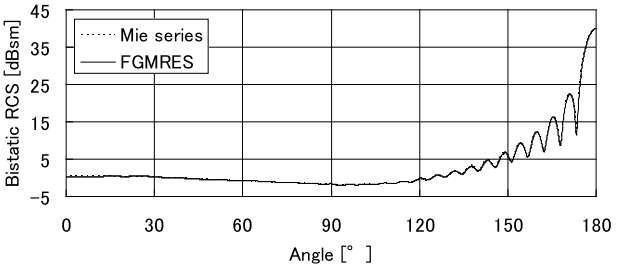
Fig. 2 displays the bistatic RCS for the dielectric-coated conducting sphere of test case (a), calculated by the inner-outer flexible GMRES and Mie series. It can be observed that inner-outer flexible GMRES agrees quite well with the Mie series for both polarizations, validating the accuracy of the solver 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_{low} and p, along with Malas' strategy [4], Fan's strategy [5], and non-preconditioned GMRES(100), and Fig. 3 compares the convergence history for the presented strategy with (L_{low}, p) = (6, 0.75), Malas' strategy [4], Fan's strategy [5], and non-preconditioned GMRES(100). From Table 2, it can be inferred that the combination (L_{low}, 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 accuracy for the FMM within the inner solver, and that a moderately accurate FMM operator is optimal. This implies that when the FMM within the inner solver is deteriorated, the inner solver can no longer serve as the preconditioner, and thus in both the cases, the total performance of the solver is not sufficiently improved. Additionally, it should be noted that the proposed strategy was proven to be superior to those of both Malas and Fan.

Table 3 lists the memory requirements for the presented strategy with (L_{low}, p) = (6, 0.75), Malas' strategy, Fan's strategy, and non-preconditioned GMRES(100). Fan's strategy needs no extra memory storage as compared to non-preconditioned GMRES since it does not take into account the far-field interaction within the inner solver, thus, the memory requirements for Fan's strategy are always equal to that for the non-preconditioned GMRES. Malas' strategy has an advantage with regard to memory utilization as compared to the proposed strategy. This is because the truncation number for FMM within the inner solver is equivalent to that for the FMM within the outer solver; therefore, the *q2M* and *L2p* translators for the outer solver can be reused for the inner solver. Consequently, Malas' strategy does not require extra memory storage for the *q2M* and *L2p* translators for the inner solver. However, the strategy does not sufficiently reduce the CPU time, as shown in Table 2. On the other hand, the proposed strategy requires a slightly larger amount of memory storage compared to other methods; however, the impact is not very significant as compared to the basic requirements for the FMM operator within the outer solver. From the observations provided, we can state that the proposed strategy with (L_{low}, p) = (6, 0.75) achieves the optimal performance with regard to the balance between the memory requirements and convergence behavior.



(a) V-V polarization



(b) H-H polarization

Fig. 2 Bistatic RCS of a dielectric-coated conducting sphere for V-V and H-H polarizations computed by inner-outer flexible GMRES and Mie series.

Table 2: Comparison of CPU time for presented strategy with various sets of L_{low} and p, along with Malas' strategy [4], Fan's strategy [5], and non-preconditioned GMRES(100); Acronyms: N.C. ≡ "not converged."

(a) Dielectric-coated conducting sphere

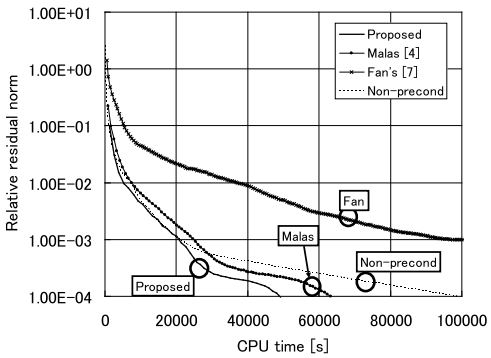
L_{low}	p	L_i	Iteration times	CPU time [s]
3	0.5	3, 4, 6, 8	200	260118.72
	0.85	3, 5, 9, 17	76	94765.04
	1.0	3, 6, 12, 24	72	61750.63
6	0.25	6, 7, 8, 10	115	140056.43
	0.55	6, 8, 12, 18	43	49121.40
	0.75	6, 10, 16, 28	40	45445.70
10	0.1	10, 10, 11, 12	N.C.	N.C.
	0.4	10, 13, 17, 22	39	51128.32
	0.58	10, 14, 22, 33	39	54802.14
Malas' [4]		10, 11, 12, 16	78	63192.40
Fan's [5]		0, 0, 0, 0	716	300452.39
Non-preconditioned GMRES(100)			1922	98959.89

(b) Dielectric-coated NASA almond

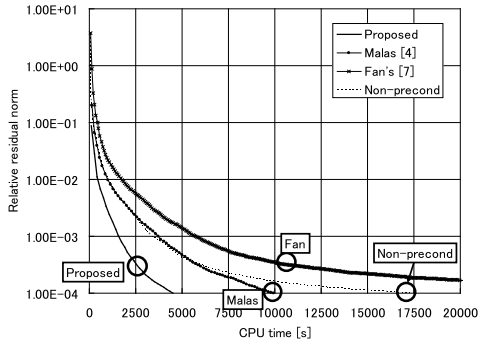
L_{low}	p	L_i	Iteration times	CPU time [s]
3	0.5	3, 4, 6, 8, 12	123	25499.16
	0.85	3, 5, 9, 17, 31	52	8840.75
	1.0	3, 6, 12, 24, 48	48	8567.96
6	0.25	6, 7, 8, 10, 12	116	21706.89
	0.55	6, 8, 12, 18, 27	29	6416.50
	0.75	6, 10, 16, 28, 48	27	4499.97
9	0.1	9, 9, 10, 11, 11	N.C.	N.C.
	0.4	9, 11, 15, 20, 27	29	6892.78
	0.58	9, 13, 20, 30, 44	27	9103.85
Malas' [4]		9, 9, 11, 13, 18	68	9927.53
Fan's [5]		0, 0, 0, 0	N.C.	N.C.
Non-preconditioned GMRES(100)			1056	17420.14

(c) FSS structure

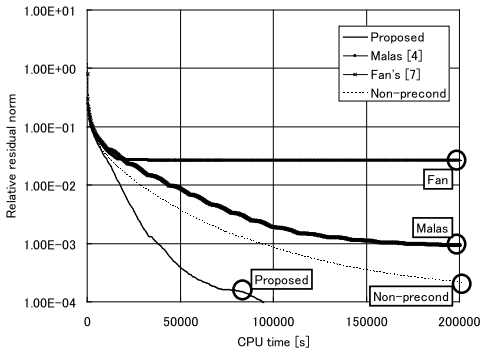
L_{low}	p	L_i	Iteration times	CPU time [s]
3	0.5	3, 4, 6, 8	N.C.	N.C.
	0.85	3, 5, 9, 17	N.C.	N.C.
	1.0	3, 6, 12, 24	225	206705.44
6	0.25	6, 7, 8, 10	N.C.	N.C.
	0.55	6, 8, 12, 18	149	113951.02
	0.75	6, 10, 16, 28	108	91884.92
10	0.1	10, 10, 11, 12	N.C.	N.C.
	0.4	10, 13, 17, 22	110	94949.39
	0.58	10, 14, 22, 33	107	99498.96
Malas' [4]		10, 11, 12, 15	N.C.	N.C.
Fan's [5]		0, 0, 0, 0	N.C.	N.C.
Non-preconditioned GMRES(100)			N.C.	N.C.



(a) Dielectric-coated conducting sphere



(b) Dielectric-coated NASA almond



(c) FSS structure

Fig. 3 Convergence history for presented strategy with (L_{low}, p) = (6, 0.75), Malas' strategy [4], Fan's strategy [5] and non-preconditioned GMRES(100).

Table 3: Comparison of the memory requirements for presented strategy with (L_{low}, p) = (6, 0.75), Malas' strategy, Fan's strategy, and non-preconditioned GMRES(100).

(a) Dielectric-coated conducting sphere

	Memory usage [GByte]
Proposed strategy with (L_{low}, p) = (6, 0.75)	46.7
Malas' strategy [4]	44.8
Fan's strategy [5]	44.7
Non-preconditioned GMRES(220)	44.7

(b) Dielectric-coated NASA almond

	Memory usage [GByte]
Proposed strategy with (L_{low}, p) = (6, 0.75)	9.09
Malas' strategy [4]	8.22
Fan's strategy [5]	8.12
Non-preconditioned GMRES(220)	8.12

(c) FSS structure

	Memory usage [GByte]
Proposed strategy with (L_{low}, p) = (6, 0.75)	25.2
Malas' strategy [4]	24.0
Fan's strategy [5]	23.9
Non-preconditioned GMRES(220)	23.9

4. 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.

Acknowledgement

All the numerical results presented in this paper were obtained from the parallel computer Express5800 which is owned by Cyberscience Center, Tohoku University, Japan.

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