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ADAPTIVELY ACCELERATED GMRES FAST FOURIER TRANSFORM METHOD FOR ELECTROMAGNETIC SCATTERING

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Abstract—The problem of electromagnetic scattering by 3D dielectric bodies is formulated in terms of a weak-form volume integral equation. Applying Galerkin's method with rooftop functions as basis and testing functions, the integral equation can be usually solved by Krylov-subspace fast Fourier transform (FFT) iterative methods. In this paper, the generalized minimum residual (GMRES)-FFT method is used to solve this integral equation, and several adaptive acceleration techniques are proposed to improve the convergence rate of the GMRES-FFT method. On several electromagnetic scattering problems, the performance of these adaptively accelerated GMRES-FFT methods are thoroughly analyzed and compared.

1. INTRODUCTION

The scattering of electromagnetic waves by objects of arbitrary shape is an important research subject. Pioneering works treating 3D arbitrary dielectric bodies are mainly based on the method of moment (MoM) [1]. MoM for this problem involves discretizing the vector volume integral equation and then solving a matrix equation with N unknowns. It is basically impractical to solve this matrix equation with a large number of unknowns using a direct solver lver because it requires $O(N^3)$ CPU time and $O(N^2)$ computer memory. Alternatively, one can solve this matrix equation by using Krylov-subspace iterative methods, which requires a reduced CPU time of $O(N^2)$ and the same computer memory.

An important improvement over the above MoM is the k-space method [2] proposed by Bojaski in the early 1980s. The k-space method uses the Krylov-subspace iterative method to solve the integral equation, and the required matrix-vector product in the iteration is efficiently evaluated by using the fast Fourier transform (FFT) technique. A large number of related papers have been reported by many researchers, which can be found in [3–8]. Among these schemes, the conjugate gradient (CG)-FFT method developed by Zwamborn and van den Berg in the 1990s leads to a weaker singularity in the dyadic Green's function and appears to be simpler to implement [3]. Recently, Liu's group developed a fast weak-form biconjugate gradient (BCG)-FFT method [4], which shows promising results because of a faster convergence speed than the conventional weak-form CG-FFT method. They further improved the convergence speed by using the weak-form discretization with the stabilized BCG (BCGS) method, which is referred to as BCGS-FFT method [5]. The combination of the Krylov-subspace iterative methods with the FFT technique reduces the CPU time to $O(N \log N)$ and computer memory to $O(N)$.

The generalized minimum residual (GMRES) method is also a kind of well-known Krylov-subspace iterative methods. Its combination with FFT technique results in the so-called GMRES-FFT method [6]. The superiority of GMRES method over other Krylov-subspace methods lies in that it only needs directly matrix-vector product operation in the iteration process and it has the property of monotonic convergence. However, the potential superlinear convergence behavior is usually inhibited since some useful historical information is believed to be lost due to restarting [9]. A few approximate eigenvectors of the coefficient matrix corresponding to the smallest eigenvalues in magnitude have been saved and used to augment the Krylov-subspace in order to mitigate this ill effect of restarting. The convergence speed of this weak-form augmented GMRES (AGMRES)-FFT [7] method is comparable to the BCG-FFT method, while the drawback of BCG-FFT is avoided. The approximate eigenvectors can also be incorporated into the Krylov-subspace by the implicit restarting scheme. The resulted GMRES with implicit restarting (GMRES-IR)-FFT method dramatically improves the convergence speed of the regular GMRES-FFT method [8].

In this paper, the GMRES-FFT method is employed to solve the weak-form volume integral equation resulting from 3D dielectric scattering problems. We focus on discussing adaptive acceleration strategies related to GMRES to enhance the performance of the

GMRES-FFT method. The outline of the paper is as follows: In Section 2, the weak-form volume integral equation for 3D dielectric scattering problems is briefly introduced. In Section 3, several acceleration techniques for GMRES are described in more details, and their theoretical properties and computational costs are analyzed and compared. Numerical performance of these accelerated GMRSE-FFT methods on several electromagnetic problems is discussed in Section 4. Finally, Section 5 provides some conclusions and comments.

2. THE VOLUME INTEGRAL EQUATION

Consider the scattering of an inhomogeneous dielectric object embedded within a finite volume V. The complex permittivity of the object is

$$\varepsilon(r) = \varepsilon_r(r)\varepsilon_0 - j\frac{\sigma(r)}{\omega} \tag{1}$$

where ε_r and σ denote the relative permittivity and the electric conductivity, respectively. Suppose the object is illuminated by an incident electric field $\mathbf{E}^i$. The volume integral equation for this problem can then be described by

$$\frac{\mathbf{D}(r)}{\varepsilon(r)} - (k_0^2 + \nabla\nabla\cdot)\mathbf{A}(r) = \mathbf{E}^i(r), \quad r \in V \tag{2}$$

with $k_0 = \omega\sqrt{\mu_0\varepsilon_0}$ and

$$\mathbf{A}(r) = \frac{1}{\varepsilon_0}\int_V G(r-r')\chi(r')\mathbf{D}(r')dr' \tag{3}$$

where $\chi(r) = \frac{\varepsilon(r)-\varepsilon_0}{\varepsilon(r)}$ and $G(r-r') = \frac{\exp(-jk_0|r-r'|)}{4\pi|r-r'|}$.

Using the weak form of the electric flux density, the electric-contrast vector potential and the incident electric field in (2) and expanding and testing the corresponding terms with 3D vector volumetric rooftop functions, a matrix equation can be obtained as the following:

$$\mathbf{Ax} = \mathbf{b} \tag{4}$$

This matrix equation can be solved efficiently by Krylov-subspace iterative methods combined with FFT technique.

In this paper, we assume that the dielectric bodies are illuminated by a x-polarized normally incident plane wave and the operating frequency is taken to be 100 MHz. The bistatic radar cross section (RCS) defined as follows:

$$\text{RCS} = 10\log(\sigma/\lambda_0^2)$$

in which

$$\sigma(\phi,\,\theta) = \lim_{R\to\infty} 4\pi R^2 \frac{\|\mathbf{E}^s(\phi,\,\theta)\|^2}{\|\mathbf{E}^i(\phi,\,\theta)\|^2}$$

Here, $\mathbf{E}^s(\phi,\,\theta)$ and $\mathbf{E}^i(\phi,\,\theta)$ denote the scattered far field and incident far-field vectors, respectively and R denotes the distance between the source point and the observed point, $\|.\|$ denotes the L_2-norm of an arbitrary vector.

3. ACCELERATION TECHNIQUES FOR GMRES

The GMRES method [9] is a popular Krylov-subspace iterative method for the solution of algebraic linear systems. In its original form, so-called full GMRES, it is optimal in the sense that it minimizes the residual over the whole Krylov-subspace. However, it is often too expensive since the required orthogonalization per iteration step grows quadratically with the number of iterations. Therefore, in practice one often uses restarted version of GMRES (GMRES (m)). In restarted GMRES method, the method is restarted once the Krylov-subspace reaches dimension m, and the current approximate solution becomes the new initial guess for the next m iterations. A disadvantage of this approach is that the convergence behavior in many situations seems to depend quite critically on the value of m. Even in situations in which satisfactory convergence takes place, the convergence is less than optimal, since the history is thrown away so that potential superlinear convergence behavior is inhibited [10]. There are many acceleration techniques that attempt to mimic the convergence of full GMRES more closely, or to accelerate the convergence of the regular GMRES by retaining some historical information at the time of restart [11–15].

Deflation methods are a main class of acceleration techniques for GMRES. It is well known that the convergence of Krylov-subspace methods depends to a large degree on the distribution of eigenvalues, and if there are small eigenvalues, then removing or deflating them can greatly improve the convergence. One way that eigenvalues can be deflated is for the corresponding eigenvectors to be in the subspace as in [7, 11], where approximate eigenvectors corresponding to the smallest eigenvalues in magnitude are saved and then added to the Krylov-subspace in the next cycle of GMRES.

A different approach for deflation is given in GMRES with implicit restarting (GMRES-IR) method [8, 12]. By using the unwanted eigenvalues as shifts for the QR iteration, it effectively restarts the GMRES with several approximate eigenvectors. However, the GMRES-IR is somewhat complicated and has stability problems associated with the implicit restarting scheme. Method proposed in [13], called GMRES with deflated restarting (GMRES-DR), uses a kind of thick restarting approach. It is mathematically equivalent to the implicit restarting. However, its implementation is simpler and it does not have the same numerical concerns.

In another approach to deflated GMRES, Kharchenko builds a spectral preconditioner for the matrix using approximate eigenvectors [14]. This spectral preconditioning technique uses approximate eigenvectors generated during only one GMRES cycle. It is improved in [15] with a method, called deflated GMRES (DGMRES) in this paper, that keeps working on the approximate eigenvectors outside of GMRES. DGMRES combines its previous approximate eigenvectors with new ones from each cycle of GMRES.

In analog to augmented GMRES (AGMRES) method proposed in [11], which augments the Krylov-subspace with approximate eigenvectors, Baker [16] observes that the residual vectors at the end of each cycle of GMRES often alternate direction in a cyclic fashion. This alternating phenomenon is simply a symptom of the lack of orthogonality between the approximate Krylov-subspace generated during the current restart cycle of GMRES and the approximate Krylov-subspaces from previous cycles. This fact indicates that faster convergence should be possible if some degree of orthogonality to previous approximate Krylov-subspaces were maintained. To achieve this goal, approximations to residual errors from previous restart cycles of GMRES are added to the current Krylov-subspace. The resulted method is called loose GMRES method (LGMRES) [16].

Another class of acceleration techniques is based on the fact that ideally the approximation Krylov-subspace should contain the correction component $\mathbf{c}$ such that $\mathbf{x} = \mathbf{x}_0 + \mathbf{c}$ is the exact solution to the problem (4). The nested Krylov-subspace method GMRES recursive (GMRESR) method [17] is one such technique. In GMRESR, the outer generalized conjugate residual (GCR) method invokes another GMRES method at each step i to approximate the solution to $\mathbf{Ac} = \mathbf{r}_i$, where $\mathbf{r}_i$ is the current residual at step i. The approximate solution to $\mathbf{Ac} = \mathbf{r}_i$ then becomes the next direction for the outer approximate space. Note that flexible GMRES (FGMRES) method [18] can also be view as a method that approximates solutions to similar residual equations at each step. Different from GMRESR method, the inner and outer iterative methods in FGMRES are both GMRES.

We now briefly look at the costs and storage requirements of these accelerated GMRES methods compared to regular GMRES method. Since the Krylov-subspace dimension m is usually far less than the number of unknowns N, only the major costs and storage for vectors of length of N are considered. The main potential advantage of GMRES-

DR and GMRES-IR compared to regular is in the convergence, and both of them also does need only m-k matrix-vector products (MVPs) per cycle while GMRES uses m, where k denotes the number of approximate eigenvectors used. Moreover, both of them can be implemented with about the same storage as GMRES. AGMRS and LGMRES are a litter higher in both expense and storage than GMRES. About k extra vectors of length N are normally used for AGMRES and LGMRES. For FGMRES and GMRESR, the costs and storage requirements almost doubles since another inner GMRES iterative method is invoked. For more details, Table 1 gives a rough count of the number of MVPs and storage of length N for one cycle of the standard restarted GMRES and the accelerated GMRES methods described above.

Table 1. The number of MVPs and storage of length N for one cycle of the regular restarted GMRES method and the accelerated GMRES methods.

Methods	GMRES	AGMRES	LGMRES	GMRES-DR
MVPs	m	$m+k$	$m+k$	m
Memory	$m+3$	$m+3k+3$	$m+3k+3$	$m+3$
Methods	GMRES-IR	DGMRES	FGMRES	GMRESR
MVPs	m	m	$2m$	$2m$
Memory	$m+3$	$m+2k+3$	$2m+m+6$	$2m+m+5$

4. NUMERICAL RESULTS AND DISCUSSIONS

The accelerated GMRES methods described in the above section can be easily combined with the FFT technique, resulting the so-call accelerated GMRES-FFT methods. In this section, these accelerated GMRES methods assumed to be combined with the FFT technique for solving linear systems arising from the discretization of the weak-form volume integral equation of electromagnetic wave scattering problems. A number of numerical results are presented to illustrate the performance of these acceleration techniques. Since the regular restarted GMRES method has been shown to be more efficient than a class of traditional Krylov-subspace methods, such as CG, BCG etc., we mainly compare the performance of the GMRES method and the proposed accelerated GMRES methods.

To demonstrate the performance of these acceleration techniques for GMRES, we re-compute the RCS of four typical dielectric geometries, which can be found in reference [8]. They consist of a homogeneous sphere with 98304 unknowns, a two-layer inhomogeneous sphere with 786432 unknowns, a cube with 98304 unknowns, and an oblate spheroid 24576 unknowns. All computations were carried out on a Pentium(R) 4 with 2.4 G CPU and 1 GB RAM in single precision. The numerical convergence is measured by the relative residual error $\|\text{current residual}\|/\|\text{initial residual}\|$. The maximum iteration number is set to be 2000 and the iteration process is terminated when the residual error falls below 10^{-3}. In all cases, a zero initial estimate is taken and the parameter $m = 30$ is chosen as the default setting. The parameter k (denotes the number of approximate eigenvectors) for AGMRES, LGMRES GMRES-DR, GMRES-IR, and DGMRES are specifically tuned in each example for optimal performance. The Krylov-subspace dimension and tolerance for inner GMRES method of both FGMRES and GMRESR are chosen as 30 and 0.01, respectively.

Figures 1–4 displays the convergence history of the accelerated GMRES methods and the regular GMRES method on the four examples. It demonstrates that all accelerated GMRES methods converge much faster than the regular restarted GMRES method on all examples. This justifies the use of acceleration techniques for GMRES method. More detailed comparisons can be found in Table 2, in which the solution cost of the accelerated GMRES methods and the regular GMRES method is evaluated in terms of number of matrix-vector products and CPU time, where $*$ refers to no convergence after maximum 2000 iterations and 's' denotes second.

It can also be found that AGMRES GMRES-DR, GMRES-

Table 2. Comparison of the solution cost for the regular GMRES method with the accelerated GMRES methods.

Examples	Sphere		Two-layer Sphere		Cube		Spheroid	
	MVPs	Time(s)	MVPs	Time(s)	MVPs	Time(s)	MVPs	Time(s)
GMRES	137	100.3	1242	884.0	1166	807.8	$*$	$*$
AGMRES	71	52.4	137	101.6	114	86.0	161	15.0
LGMRES	91	68.7	200	151.4	275	212.1	448	42.0
GMRES-DR	63	43.5	125	84.8	112	77.2	136	12.0
GMRES-IR	63	57.2	109	99.3	112	105.9	148	19.8
DGMRES	64	44.0	127	90.8	126	91.5	159	13.5
FGMRES	108	74.2	263	180.1	331	231.4	303	23.9
GMRESR	108	73.2	232	157.9	300	207.5	303	23.8

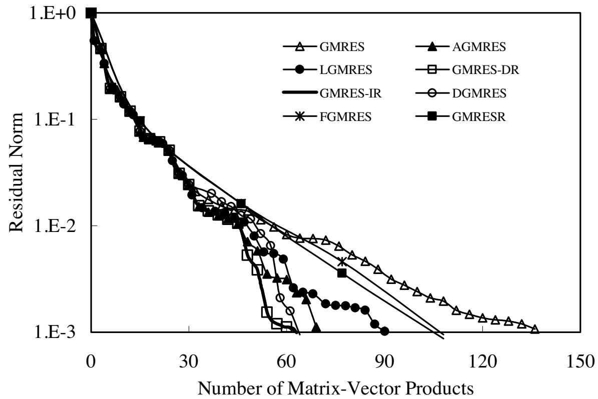

Figure 1. The convergence history of the regular GMRES method and the accelerated GMRES methods on the homogeneous sphere example.

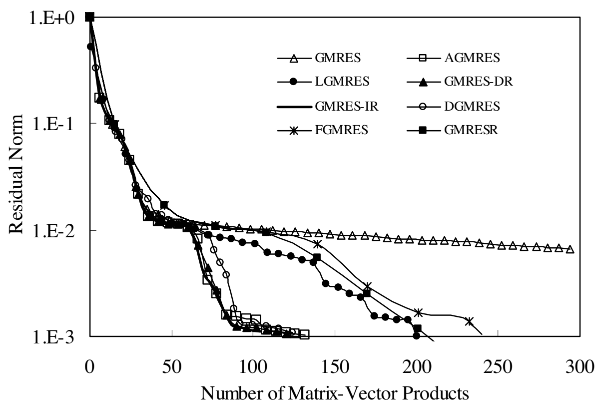

Figure 2. The convergence history of the regular GMRES method and the accelerated GMRES methods on the inhomogeneous two-layer sphere example.

DR and DGMRES methods can converge much faster than other accelerated GMRES methods. This demonstrates the efficiency of the kind of deflation technique for GMRES method when solving electromagnetic scattering problems. Moreover, these four accelerated GMRES methods exhibit similar convergence curve. This is because they belong to the same class of acceleration techniques although they use approximate eigenvectors to deflated eigenvalues in different ways. At the same time, since the eigenvector information is incorporated in the Krylov-subspace from the beginning instead of being appended at the end of the cycle as done in AGMRES, GMRES-DR and GMRES-IR obtain a faster convergence rate than AGMRES. Since GMRES-DR and GMRES-IR methods are mathematically equivalent to each other, they almost give the same convergence curve.

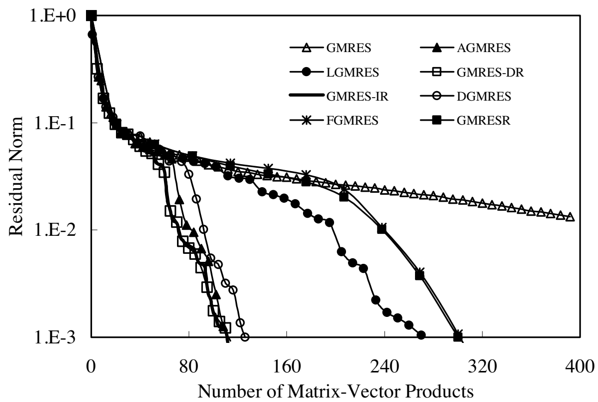

Figure 3. The convergence history of the regular GMRES method and the accelerated GMRES methods on the cube example.

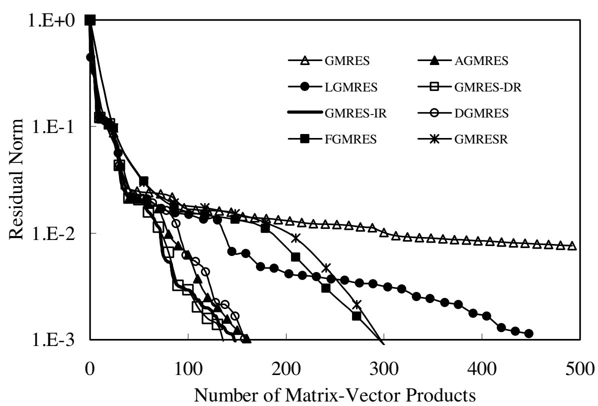

Figure 4. The convergence history of the regular GMRES method and the accelerated GMRES methods on the oblate spheroid example.

Instead of deflating smallest eigenvalues by use of approximate eigenvectors as AGMRES, LGMRES augments the Krylov-subspace with approximations to the residual errors at each end of cycle, in order to maintain the orthogonality between previous Krylov-subspaces.

Although the convergence speed of LGMRES method is much slower than that of AGMRES as shown in Figs. 1–4, its implementation is more simpler and the approximations to the residual errors can be easily obtained from the GMES method without any additional cost.

As shown in Figs. 1–4, FGMRES and GMRESR methods can decrease dramatically the number of outer iterations of GMRES and GCR, respectively, by use of another GMRES method as an inner iterative method. However, the introduction of the inner GMRES method also consumes much computational costs. And the overall convergence improvement depends on the balance of the acceleration effect and the added computational cost [19–28].

5. CONCLUSIONS

In this paper, the kind of GMRES-FFT method is proposed for the iterative solution of 3-D volume electric field integral equation of 3-D dielectric electromagnetic scattering problems. In order to improve the convergence of GMRES-FFT method, several acceleration techniques are overviewed and compared. Numerical results demonstrate that these acceleration techniques can significantly speed up the convergence rate of GMRES-FFT method. Among these acceleration techniques, both GMRES-DR and GMRES-IR methods are the most efficient and robust when 3-D dielectric electromagnetic scattering problems are considered.

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