

FLEXIBLE GMRES SOLVER FOR BOUNDARY ELEMENT ANALYSIS OF ACOUSTIC FIELDS

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This paper presents an iterative solution strategy for boundary element analysis of acoustic field problems based on flexible GMRES method. A recently proposed formulation for higher order elements has been used for boundary element discretization, which employs Burton-Miller approach at interior nodes and the normal derivative integral equation at the corner nodes of a quadratic element. Resulting linear system is solved using an inner-outer GMRES iterative scheme in which the outer iteration corresponds to the flexible GMRES method. The inner iterations correspond to the GMRES method and provide a right preconditioner for the outer flexible GMRES iteration. Numerical results have been obtained using fully assembled boundary element system matrix. The present implementation essentially forms the first step in our ongoing research on development of a fast iterative solver for the recent boundary element formulation for higher order elements.

Keywords: Boundary element method; acoustics; Helmholtz equation; flexible GMRES

1. Introduction

The boundary element method (BEM) offers an attractive alternative to domain discretization methods (FEM, FVM, FDM) for solution of acoustic problems. BEM is especially attractive for exterior acoustic problems since it implicitly fulfills the Sommerfield radiation condition. Reduction of dimensionality provided by BEM tremendously simplifies the pre-processing step involving modeling and grid generation. However, the traditional BEM has a serious disadvantage vis-à-vis FEM for large-scale practical problems. The boundary element discretization yields a dense indefinite system matrix, which results in cost and memory requirement of $O(N^2)$ in the number of unknowns as compared to $O(N)$ requirement of finite element techniques. Thus, the recent boundary element research has been focused on fast iterative solvers, which can alleviate this problem [1-11]. Most of these developments are based on Krylov subspace iterative solvers [12] in conjunction with appropriate preconditioners and fast multipole method for evaluation of matrix-vector products, which reduce the memory as well as computational complexity from $O(N^2)$ to $O(N \log^\alpha N)$ where $\alpha \geq 1$ is a small positive number. Amongst Krylov subspace solvers for general linear systems, the generalized minimum residual method (GMRES) [13] has emerged as the most robust iterative solver [14].

For exterior problems (or interior problems containing subdomains), special care is required in the integral equation formulation. Use of the standard boundary integral formulation does not yield a unique solution for this class of

problems at resonance frequencies of the associated interior problem. Two different approaches have been adopted to ensure uniqueness of the numerical solution. The first one (Schenk [15]) employs additional collocation points in the domain. The second approach (due to Burton and Miller [16]) uses a linear combination of the standard and the hyper-singular (normal derivative) boundary integral equations. A variant of the Burton-Miller approach has been recently proposed by Tanaka et al. [17,18] for higher order elements. This new formulation employs the combined integral equation (Burton-Miller approach) at the interior nodes of a quadratic element and only the normal derivative boundary integral equation at the extreme (corner) nodal points. This approach ensures the uniqueness of the solution and also provides considerable reduction in the number of evaluations of boundary integrals and kernel functions as compared to the Burton-Miller formulation. Thus, this new formulation would improve the computational efficiency of the boundary element method for acoustic field analysis.

Boundary element implementation of Tanaka et al. [17,18] is based on direct solution of the boundary element system, which precludes its applicability to large-scale problems. The present work is a part of on-going effort to develop a fast solver for this formulation which involves two distinct tasks: (i) an iterative solver based on GMRES method with an appropriate preconditioner, and (ii) extension of fast multipole method for matrix-vector products. We focus on the first task in this paper. The second part, which would complete the implementation of the fast solver, would be reported later.

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We note that most of the existing fast multipole boundary element (FMBEM) implementations are based on constant elements. Although the conceptual framework of FMBEM remains the same for any element and problem type, details and complexity of implementation vary considerably. Thus, the available details in the literature would require considerable extension for FMBEM implementation of the new boundary element formulation, which exclusively involves quadratic (or higher order) elements.

We present a brief review of the new boundary integral formulation in the next section. This is followed by an overview of the iterative solver based on the flexible GMRES method, sample numerical results and concluding remarks.

2. Boundary integral formulation

For time harmonic behavior, the pressure p in an acoustic field is governed by the Helmholtz equation

$$\nabla^2 p(x) + k^2 p(x) + f(x) = 0 \quad (1)$$

where k is the wave number and f is the source term. For exterior problems, the Helmholtz equation (1) is solved in the domain Ω^c which is the complement to the open set $\Omega \subset \mathbb{R}^3$ with boundary $\Gamma = \Gamma^N \cup \Gamma^D$. On the Dirichlet boundary Γ^D , acoustic pressure is prescribed as

$$p(x) = \bar{p}(x), \quad x \in \Gamma^D \quad (2)$$

On the Neumann boundary Γ^N , acoustic flux is given as

$$q(x) = \frac{\partial p}{\partial n} = \bar{q}(x), \quad x \in \Gamma^N \quad (3)$$

Application of regularized boundary integral formulation to Helmholtz equation (1) yields the ordinary boundary integral equation (OBIE) [17]:

$$\begin{aligned} & \int_{\Gamma} \{ \dot{q}^*(x, y) - \dot{Q}^*(x, y) \} p(x) \, d\Gamma(x) \\ & + \int_{\Gamma} \dot{Q}^*(x, y) \{ p(x) - p(y) \} \, d\Gamma(x) \\ & = -i\omega\rho \int_{\Gamma} p^*(x, y) v(x) \, d\Gamma(x) + I p^*(x^s, y) \end{aligned} \quad (4)$$

where $p^*(x, y)$ is the fundamental solution of the Helmholtz equation and $\dot{q}^*(x, y)$ is its normal derivative; $\dot{Q}^*(x, y)$ is the normal derivative of the fundamental solution for Laplace equation; I is the intensity of the point sound source and $v(x)$ is the velocity related to the acoustic flux by $q(x) = -i\omega\rho v(x)$, ρ being the air density.

Taking the normal derivative of eq.(4) at the source point y results in the following normal derivative boundary integral equation (NDBIE)[17]:

$$\begin{aligned} & \int_{\Gamma} \{ \ddot{q}^*(x, y) - \ddot{Q}^*(x, y) \} p(x) \, d\Gamma(x) \\ & + \int_{\Gamma} \ddot{Q}^*(x, y) \{ p(x) - p(y) - r_m(x, y) p_{,m}(y) \} \, d\Gamma(x) \\ & = -i\omega\rho \int_{\Gamma} \{ \ddot{p}^*(x, y) - \ddot{u}^*(x, y) \} v(x) \, d\Gamma(x) \\ & - i\omega\rho \int_{\Gamma} \ddot{u}^*(x, y) \{ v(x) - n_m(x) p_{,m}(y) \} \, d\Gamma(x) \\ & + I \ddot{p}^*(x^s, y) \end{aligned} \quad (5)$$

In the preceding equation, for a function z , $\ddot{z} \equiv \partial z / \partial n(y)$, $r_m = x_m - y_m$, n_m is the component of unit normal in direction m , and u^* is the fundamental solution to the Laplace equation.

Equations (4) and (5) can be rewritten in the following compact form using operator notation:

$$\text{OBIE: } (Kp)(y) + (Vv)(y) = b(y) \quad (6)$$

$$\text{NDBIE: } (Dp)(y) + (K'v)(y) = b'(y) \quad (7)$$

Both the OBIE (6) and NDBIE (7) fail to yield a unique solution if the frequency corresponds to an eigenfrequency of the associated interior problem. Burton and Miller [13] showed that a linear combination of (6) and (7) (CBIE) yields a unique solution for all the frequencies. Tanaka et al. [17,18] propose a new method that does not apply the linear combination at all nodes of a quadratic element. They instead propose to use (a) Burton-Miller approach (CBIE) at the end points (or corner nodes) and the scaled NDBIE at the rest of the nodes [17], or (b) Burton-Miller approach (CBIE) at middle and NDBIE at corner nodes [18]. Both the options have been shown to yield a unique solution, and require fewer boundary integral and kernel function evaluations as compared to the usual Burton-Miller approach. Of these, option (b) has been observed to be slightly more efficient than option (a) and is summarized in the following box:

NEW BIE FORMULATION [18]

- If the source point is an interior node, use the **CBIE**

$$\begin{aligned} & [(Kp)(y) + (Vv)(y)] + \frac{i}{k} [(Dp)(y) + (K'v)(y)] \\ & = b(y) + \frac{i}{k} b'(y) \end{aligned} \quad (8)$$

- Else if the source point is a corner node, use the **scaled NDBIE**

$$\frac{i}{k} [(Dp)(y) + (K'v)(y)] = \frac{i}{k} b'(y) \quad (9)$$

In the preceding equations, i/k is the coupling parameter chosen to yield a favorable condition number and has been shown to be quasi-optimal by Kress [19].

3. Iterative solution of boundary element system

Boundary element discretization leads to a linear system

$$\mathbf{Ax} = \mathbf{b} \quad (10)$$

The system matrix \mathbf{A} is fully populated, non-Hermitian and indefinite. Hence, the direct solution of eq.(10) is not feasible for large-scale problems because of the prohibitive memory and computing time requirements. Thus, iterative solution of (10) is the only viable option.

3.1 Generalized minimal residual method (GMRES)

Various iterative methods are available for solution of large linear systems. Of these, Krylov subspace methods [12] are the most-suitable iterative solvers for the boundary element system (10). The generalized minimal residual method

(GMRES)[13] has emerged as the most robust and appropriate choice amongst the Krylov subspace methods. Various black-box implementations of GMRES are available in public domain, which can be easily tailored for use with a boundary element program. In the present work, we have opted for the GMRES implementation of Frayssse et al. [20,21] which is based on the reverse communication mechanism for matrix-vector products and preconditioning, and thus, provides a very flexible interface for its integration with the user-specific program. Full details of the GMRES algorithms and guidelines for the use of the routines based on them can be found in Frayssse et al. [20,21].

3.2 Approximate inverse preconditioner

The rate of convergence of any Krylov subspace method is dependent on the choice of the preconditioner. Various preconditioners have been tried for the boundary element system for acoustic problem including incomplete LU decomposition and approximate inverse preconditioners. Approximate inverse methods are generally less prone to instabilities on indefinite systems, and hence, preferred in boundary element analysis. The construction of the approximate inverse preconditioner is normally based on the operator splitting taking advantage of the rapid decay of the Green's function [5]. The integral operator A (which corresponds to the system matrix \mathbf{A}) can be split as

$$A = A_0 + \tilde{A} \quad (11)$$

where A_0 represents a bounded contribution and \tilde{A} is the remaining part. The choice of the sparsity pattern has a strong influence on the convergence of the iterative solver. Carpentieri et al. [22] discuss the effective of various sparse selection strategies in the context of electromagnetic problems. Typically, the operator A_0 is constructed by considering a layer of elements Γ_0 around a source point [22,23]. Although the operator A_0 is sparse, exact application of A_0^{-1} would be too expensive. Hence, an approximate inverse of A_0 is computed based on Frobenius norm minimization (i.e. $\min \|\mathbf{I} - \mathbf{A}\mathbf{M}\|_F$) to obtain the approximate inverse preconditioner matrix \mathbf{M} . Frobenius norm is chosen since it allows the decoupling of the constrained minimization problem into N independent linear least squares problems using the identity

$$\min \|\mathbf{I} - \mathbf{A}\mathbf{M}\|_F^2 = \sum_{j=1}^N \min \|\mathbf{e}_j - \mathbf{A}\mathbf{m}_j\|_2^2 \quad (12)$$

where \mathbf{m}_j is the column vector representing the j_{th} column of \mathbf{M} , and \mathbf{e}_j is the j_{th} canonical unit vector. The construction of the preconditioner can be further simplified by using the sparse approximation \mathbf{A}_0 based on the sparsity pattern S_j . For each source point j , $S_j = \{j_1, j_2, \dots, j_n\}$ contains all the nodes in Γ_0 . For ordering S_j , let us assume that $j_1 = j$, then the least squares problem

$$\min \|\mathbf{e}_j - \mathbf{A}\mathbf{m}_j\|_2, \quad j = 1, \dots, N \quad (13)$$

is equivalent to solving the linear systems [24,25]

$$\begin{pmatrix} a_{j_1 j_1} & a_{j_1 j_2} & \dots & a_{j_1 j_n} \\ a_{j_2 j_1} & a_{j_2 j_2} & \dots & a_{j_2 j_n} \\ \vdots & \vdots & \ddots & \vdots \\ a_{j_n j_1} & a_{j_n j_2} & \dots & a_{j_n j_n} \end{pmatrix} \begin{pmatrix} m_{j_1} \\ m_{j_2} \\ \vdots \\ m_{j_n} \end{pmatrix} = \begin{pmatrix} 1 \\ 0 \\ \vdots \\ 0 \end{pmatrix}, \quad j = 1, N \quad (14)$$

The solution vectors $\mathbf{m}_j = (0, \dots, m_{j_1}, m_{j_2}, \dots, m_{j_n}, 0, \dots, 0)^T$ of the N systems (14) set up the approximate inverse preconditioner \mathbf{M} .

The preceding approach for constructing the approximate inverse preconditioner is particularly useful in the context of the FMBEM where all the entries of the system matrix \mathbf{A} are not available and its sparse approximation \mathbf{A}_0 can be formed from the near-field part of the matrix which is explicitly computed.

3.3 Flexible GMRES method

The GMRES solver with sparse approximate inverse preconditioner performs very well [5,23,24]. At the same time, in the context of FMBEM, it is possible to construct efficient preconditioners, which also use the FMM [9]. One such possibility would be to use GMRES itself to form a preconditioner. However, such a preconditioner would be essentially nonlinear, whereas the preconditioner for a Krylov subspace solver such as GMRES must represent the same linear operator in each iteration. A method that is free from the preceding restriction is known as the flexible GMRES (FGMRES) [26], which essentially consists of inner-outer iterations. The outer iterations correspond to the right-preconditioned flexible GMRES iterations. The inner iterations correspond to the standard GMRES iterations, which may be preconditioned.

Using the GMRES and FGMRES implementations of Frayssse et al. [20,21], we have developed an interface routine, which can be easily integrated with any BEM or FMBEM implementation. This interface provides the option of separate specification of all the parameters — tolerance, maximum number of iterations, projection size etc. — and user-specified routines for matrix-vector products for outer FGMRES and inner GMRES iterations. Workspaces required by FGMRES and GMRES are allocated dynamically based on the projection size of the respective Krylov subspaces.

Instead of using a fixed tolerance for the inner iterations, one can use a variable tolerance linked to the state of convergence of the outer FGMRES iteration [10]. Such a scheme would ensure that the inner linear system is not solved more accurately than what remains to be achieved in the outer iteration. Giraud et al. [10] suggest the following expression for the tolerance of the inner iteration at the k -th FGMRES iteration

$$\varepsilon_{\text{inner}}^{(k)} = \varepsilon_{\text{outer}}^{(k)} \|\mathbf{b}\|_2 / \left(2 \|\mathbf{r}_k^{\text{FGMRES}}\|_2 \right) \quad (15)$$

where \mathbf{r}_k denotes residual at k -th iteration. Use of the preceding relation would ensure that the inner GMRES iterations adapt to the outer FGMRES scheme. The accuracy requested for the inner scheme is relaxed with the convergence of FGMRES iterations, which should improve the computational efficiency of the solution process. The outline of the FGMRES solver is given in the following box.

FLEXIBLE GMRES SOLVER

1. Set tolerance ε and initial guess \mathbf{x}_0
2. begin FGMRES
3. Compute $\mathbf{r}_0 = \mathbf{b} - \mathbf{A}\mathbf{x}_0$; $\beta = \|\mathbf{r}_0\|$; $\mathbf{v}_1 = \mathbf{r}_0 / \beta$.
4. for $k = 1, 2, \dots$, maxiter do // FGMRES iteration
5. // GMRES as right preconditioner for FGMRES
6. begin GMRES // Solve $\mathbf{A}\mathbf{z}_k = \mathbf{v}_k$ using GMRES
7. Compute $\varepsilon_{\text{inner}}$, $\mathbf{r}'_0 = \mathbf{v}_k$; $\beta' = \|\mathbf{r}'_0\|$; $\mathbf{v}'_1 = \mathbf{r}'_0 / \beta'$.
8. for $l = 1, 2, \dots, m$ do // GMRES iterations
9. $\mathbf{z}'_l = \mathbf{M}\mathbf{v}'_l$ // Preconditioner for GMRES
10. Generate basis, Hessenberg matrix, etc.
11. Exit if convergence detected
12. end for
13. end GMRES (return \mathbf{z}_k)
14. Generate Arnoldi basis, Hessenberg matrix etc.
15. Solve least squares problem
16. $\min \|\beta \mathbf{e}_1 - \bar{\mathbf{H}}_k \mathbf{y}\|$ for \mathbf{y}
17. Exit if convergence is detected.
18. end for
19. end FGMRES (return $\mathbf{x} = \mathbf{x}_0 + \mathbf{Z}_m \mathbf{y}$)

4. Numerical Results

To assess the performance of the flexible GMRES method for the solution of the boundary element system arising from the new formulation, we consider its application to two representative problems. The first problem is an exterior problem, whereas the second one represents an interior problem containing a subdomain. Following parameters have been used for the flexible GMRES iteration:

- Size of the Krylov subspace, $m = 50$
- Tolerance for convergence, $\varepsilon_{\text{outer}} = 1.0\text{d-}06$
- Maximum number of iterations, maxiter = 1000

Parameters for the inner GMRES iterations are:

- Size of the Krylov subspace, $m_2 = 20$
- Tolerance for convergence, $\varepsilon_{\text{inner}} = 5.0\text{d-}02$
- Maximum number of iterations, maxiter2 = 20

For both problems, flexible GMRES runs were made with and without preconditioned inner GMRES iterations. However, the sparse approximate inverse preconditioner constructed using a single layer of elements did not work. Hence, we report the results obtained with unpreconditioned inner GMRES.

4.1 Breathing sphere problem

We compute the acoustic field in the exterior region of a sphere of radius 0.2 m. The surface of the sphere is vibrating with a velocity $v = 1.0$ m/s. Exploiting the symmetry with respect to the coordinate planes, we model 1/8th of the sphere. Quadratic elements have been used for discretization of the sphere surface (total number of elements = 288, number of nodes = 868). Thus, the size of the boundary element system, $N = 868$.

Results for sound pressure levels for different frequencies are presented in Table 1. These are almost identical to those obtained with the direct solver, and thus,

confirm the correctness of the flexible GMRES solver. Table 2 lists the CPU time required for the solution of the linear system with the direct solver and the flexible GMRES method. For this small-size problem, the direct solver is nearly twice as fast as the flexible GMRES.

Table 1: Breathing sphere problem: comparison of sound pressure level computed with the flexible GMRES and the direct solvers.

Frequency	Sound pressure level	
	Direct solver	Flexible GMRES
1	187.1004	187.1005
2	181.0797	181.0797
4	175.0584	175.0584
8	169.0352	169.0352
20	161.0579	161.0579

Table 2: Breathing sphere problem: comparison of computation time for the flexible GMRES and the direct solvers.

Frequency	CPU Time in sec. (Iterations)	
	Direct solver	Flexible GMRES
1	4.0625	8.15625 (25)
2	4.03125	7.53125 (23)
4	4.03125	7.84375 (24)
8	4.03125	7.21875 (22)
20	4.03125	6.59375 (20)

4.2 Interior problem

We compute the acoustic field in the interior region between two concentric spheres. The radii of the inner and outer spheres are 0.1 m and 0.25 m respectively. The surface of the inner sphere is vibrating with a velocity $v = 1.0$ m/s. A total of 288 quadratic elements have been used for discretization of the spherical surfaces (number of nodes = 868). Thus, the size of the boundary element system, $N = 868$, which is the same as in the previous example.

Results for sound pressure levels for different frequencies are presented in Table 3. Once again, FGMRES results are identical to those obtained with the direct solver. Table 4 lists the CPU time required for the solution of the linear system with the direct solver and the flexible GMRES. Once again, the direct solver is nearly twice as fast as the flexible GMRES.

Table 3: Interior problem: comparison of sound pressure level computed with the flexible GMRES and the direct solvers.

Frequency	Sound pressure level	
	Direct solver	Flexible GMRES
1	106.9174	106.9174
2	110.3641	110.3641
4	132.4414	132.4414
8	138.4382	138.4382
20	121.7339	121.7339

Table 4: Interior problem: comparison of computation time for the flexible GMRES and the direct solvers.

Frequency	CPU Time in sec. (Iterations)	
	Direct solver	Flexible GMRES
1	3.9375	6.5937 (20)
2	3.8594	5.7031 (17)
4	3.8594	6.0000 (18)
8	3.7812	10.0468 (31)
20	3.7812	6.5937 (20)

For both of these small-size problems, the direct solver is nearly twice as fast as the flexible GMRES. At the same time, let us keep in mind that the present boundary element implementation is based on the dense matrix-vector product for GMRES iterations (inner as well as outer iterations). Given the small number of iterations required by the flexible GMRES, we can expect an order of magnitude improvement in the computational efficiency the iterative solver if the matrix-vector product can be computed using fast-multipole expansions, in which we can use a higher order expansion for accurate evaluation of the matrix-vector products in the outer (FGMRES) iterations and a lower order (less accurate) one in the inner (GMRES) iteration.

There are quite a few parameters and choices, which may potentially affect the performance of the FGMRES method. Size of the Krylov subspace is the most fundamental parameter. Table 5 presents the effect of variation of sizes of the Krylov subspaces of flexible GMRES (m) and inner GMRES (m_2) on the overall performance of the FGMRES method for the second problem. Results are included for a single frequency (trend is very similar at other frequencies as well). For the given value of $N = 868$, a very small value of either of the parameters leads to slower convergence. A moderate value of $m (\geq 20)$ together with $m_2 = 15$ would be the optimum choice.

Table 5: Interior problem: performance of FGMRES with varying sizes of Krylov subspaces.

FGMRES m	Iterations with size of inner GMRES			
	$m_2 = 5$	$m_2 = 10$	$m_2 = 15$	$m_2 = 20$
10	71	54	30	30
20	37	20	18	20
30	29	20	18	20
40	29	20	18	20
50	29	20	18	20

5. Concluding remarks

We have presented a flexible GMRES for boundary element analysis of acoustic field problems based on a new boundary integral formulation for higher order elements. Resulting linear system is solved using an inner-outer GMRES iterative scheme in which the outer iteration corresponds to the flexible GMRES method. The inner iterations correspond to the GMRES method and provide a right preconditioner for the outer flexible GMRES iteration. Numerical results have been obtained using fully assembled boundary element system matrix. The present work essentially forms the first step in FMBE implementation of

the new boundary element formulation for higher order elements.

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