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On the Choice of Krylov Methods and Preconditioners for a Domain Decomposed Iterative Solution of the Exterior Helmholtz Problem

Antonini Puppin Macedo [1]

Introduction

From a finite element viewpoint, the solution of the Helmholtz problem has stability problems related to its operator, in particular the loss of ellipticity for high wave numbers. Regardless of the stability properties of the finite element method used in its discretization, the Helmholtz problem requires always a minimal number of elements per wave length to correctly represent the physical phenomena and to avoid an under-resolved numerical solution. The engineering literature often refers to 10 elements per wave length $kh = \pi/5$ as providing an acceptable resolution. Therefore realistic scattering problems intrinsically require fine meshes leading to significantly large-scale systems of equations that must be solved to high precision in engineering applications.

It is also important to note that the finite element discretization of the Helmholtz operator results in systems which combine stiffness and mass terms in the form,

$$[\mathbf{K} - k^2\mathbf{M}]\mathbf{u} = \mathbf{f} \tag{1}$$

that is symmetric and *indefinite* for high wave numbers. Also, for the exterior Helmholtz problem, the Sommerfeld operator adds a contribution of a general form $ik\mathbf{M}_S$ to the system matrices resulting in a system often called complex, symmetric and indefinite. We note that $\mathbf{M}_S$ is a mass matrix restricted to the dof's on the external boundary.

1 Department of Aerospace Engineering Sciences, and Center for Aerospace Structures, University of Colorado at Boulder, Boulder, CO 80309-0429, U. S. A.
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Domain decomposition - DD - methods for such problem in general lead to systems with the same characteristics, which poses several challenges for their development. In this context, the recent DD literature is very rich in relevant contributions to the solution of the exterior Helmholtz problem [Des90, BD96, CCEW98, dLBFM$^+$98, FML98a, FML$^+$98b]. Among these works the so-called FETI-H method [FML98a, FML$^+$98b] is one of the most efficient for large scale systems. This method is a dual Schur complement method that comes from a modified Lagrangian operator using Lagrange multipliers to enforce continuity between subdomains, resulting in an interface problem that is solved by means of iterative Krylov methods. These systems, as a result of the use of dual Schur complements, are very ill-conditioned degrading convergence. To solve this complex, symmetric, indefinite and ill-conditioned systems we intend to investigate the application of well-known algorithms for the Helmholtz operator, namely: Conjugate Residuals - CR -, Generalized Conjugate Residuals - GCR -, Bi-conjugate Gradients - BCG - and Generalized Minimal Residual - GMRES.

This paper is organized as follows. In section 2, we present the system of interface equations resulting from the FETI-H method. In section 3, we discuss the iterative solution of this system and appropriate preconditioners. We end the paper with a series of numerical experiments.

The regularized FETI method for complex problems

The Euler equations associated with the FETI-H modified Lagrangian can be written as (see [FML98a, FML$^+$98b] for more details):

$$(\widetilde{\mathbf{K}}^s + ik\mathbf{M}_I^s)\mathbf{u}^s = (\mathbf{K}^s - k^2\mathbf{M}^s + ik\mathbf{M}_I^s)\mathbf{u}^s = \mathbf{f}^s - \mathbf{B}^{s^T}\lambda \tag{2}$$

$$\sum_{s=1}^{s=N_s} \mathbf{B}^s\mathbf{u}^s = 0 \tag{3}$$

where

$$\mathbf{M}_I^s = \begin{bmatrix} 0 & 0 \\ 0 & \sum_{\Omega^s \cap \Omega^q \neq \{\emptyset\}} \epsilon^{s,q}\mathbf{M}_{bb}^{s,q} \end{bmatrix} \tag{4}$$

and it follows that $\mathbf{M}_I^s$ has a constant sign within a subdomain and opposite sign in its neighbors, that is, if $\forall q/\Omega^s \cap \Omega^q \neq \{\emptyset\}$ $\epsilon^{s,q} = 1$, so $\forall s/\Omega^q \cap \Omega^s \neq \{\emptyset\}$ $\epsilon^{q,s} = -1$ or both $\epsilon^{q,s}$ and $\epsilon^{s,q}$ are set to zero. Note that in [FML98a] it is shown that a modified Lagrangian approach ensures that the resulting subdomain problem matrices $\widetilde{\mathbf{K}}^s + ik\mathbf{M}_I^s$ are always non singular and an algorithm is proposed to ensure that the signing condition imposed by $\epsilon^{s,q}$ is always satisfied and at least one edge of each subdomain has a non-zero ϵ.

From (3), we find that the interface problem associated with the regularized subdomain equations (2) is given by

$$\mathbf{F}_I\lambda = \mathbf{d} \tag{5}$$

where

$$\mathbf{F}_I = \sum_{s=1}^{s=N_s} \mathbf{B}^s(\mathbf{K}^s - k^2\mathbf{M}^s + ik\mathbf{M}_I^s)^{-1}\mathbf{B}^{s^T}$$

$$\mathbf{d} = \sum_{s=1}^{s=N_s} \mathbf{B}^s(\widetilde{\mathbf{K}}^s + ik\mathbf{M}_I^s)^{-1}\mathbf{f}^s$$

where $\mathbf{B}$ is a signed boolean matrix that extracts the boundary components from a subdomain vector, $\mathbf{M}_I$ is the "interface mass" emanating from the modified Lagrangian of the FETI-H method (see [FML98a]).

The performance of iterative solvers for this system is then crucial in FETI type methods and the efficiency of the Krylov methods used will play a significant rule. Recalling the discussion in the introduction, this system presents challenging difficulties that has required the development of preconditioning techniques that make the solution by Krylov methods feasible. In the next section, we discuss the appropriate Krylov methods for this problem as well as the development of preconditioning techniques at both coarse and local levels for the FETI-H method.

Iterative solution of the interface problem

For the iterative solution of complex systems emanating from the Helmholtz discretization, we intend to focus on basically two approaches. First, methods that take advantage of the symmetry of the problem are considered, namely the Conjugate Residuals - CR - and the Bi-Conjugate Gradients - BCG - algorithms. Because of this, the inner product used for these solvers is redefined from what is expected for complex systems and the requirement of a full-reorthogonalization for the search directions is circumvented. Second, methods traditionally well regarded for the solution of indefinite systems are considered, but in this case they require full reorthogonalization of the search directions, as in the Generalized Conjugate Residuals - GCR - and the Generalized Minimal Residuals - GMRES - algorithms. [2]

The BCG algorithm, derived from the Lanczos recursion, is a Conjugate Gradient like method and will be implemented in its transpose-free version [Fre92]. [3]

The CR algorithm, on the other hand, is derived from GMRES in the particular case of a symmetric system matrix $\mathbf{A}$. In this case, the residual vectors should be $\mathbf{A}$-orthogonal, i.e., they are conjugate (hence the name of the algorithm). In addition, the search directions $\mathbf{p}$, are also $\mathbf{A}$ orthogonal. The resulting algorithm has the same structure as the standard Conjugate Gradients algorithm, but satisfies these conditions and requires only one more vector update, i.e., $2n$ more operations, than CG [Saa95].

A very important point related to the application of these algorithms is that the definition of the inner-product must be redefined as:

$$(\mathbf{x}, \mathbf{y}) \;=\; \mathbf{y}^T\mathbf{x}, \qquad \mathbf{x}, \mathbf{y} \;\in\; \mathcal{C}^n \tag{6}$$

for *symmetric* complex matrices, and not as

$$(\mathbf{x}, \mathbf{y}) \;=\; \mathbf{y}^H\mathbf{x}, \qquad \mathbf{x}, \mathbf{y} \;\in\; \mathcal{C}^n \tag{7}$$

as normaly used for complex matrices. See [Cra69, Fre92, Mac99] for a deeper discussion on this.

The other algorithms we intend to apply to this problem, GCR and GMRES, require a full reorthogonalization of the search directions in their standard form. For the Helmholtz problem, within the current framework, the number of iterations may become very large and the storage and computational requirements may become impractical. The literature is rich in restarted and truncated versions, but they are well known to stagnate when the matrix

2 Because of the page limit for this contribution, we refer the reader to [Saa95, Fre92, Mac99] for a detailed description of these algorithms.

3 In [ZW94], we find that the iterations of another well regarded solver for Helmholtz problems, the Quasi-Minimal Residuals - QMR - algorithm, can be obtained from those of BCG as a particular case of residual smoothing.

is not positive definite. In our numerical experiments, large scale problems have a strong tendency to stagnate for all algorithms, even when full reorthogonalization is used. The use of preconditioning techniques is an obvious option to keep the number of iterations small making it feasible to use any method.

For the FETI-H method the development of a two-level coarse projection approach (see [FML98a, FML$^+$98b] for details) represent the a most crucial point in the high performance of the method, combined with the modified Lagrangian formulation that *per se* provides scalability with respect to the element size as well as guarantees that the local subdomain problems are solvable. In addition, we propose efficient local preconditioning techniques that will improve convergence even more. We will compare the performance of the different algorithms. To make this paper self-contained, we briefly present the coarse projection technique in the next section and we then discuss the ideas of the local preconditioner.

A coarsening strategy: the improved FETI-H algorithm

The idea of the coarse projection is, in fact, the main characteristic of the FETI-H method. It basically accelerates convergence by modifying the Krylov iterations by enforcing the following *optional admissible constraint* on the residuals $\mathbf{r}^k$ in each iteration:

$$\mathbf{Q}^T\mathbf{r}^k \;=\; 0\;. \tag{8}$$

Here $\mathbf{Q}$ is a coarse subspace containing a set of plane waves (see [FML98a, FML$^+$98b] for details). This leads to the following projector:

$$\mathbf{P} \;=\; \mathbf{I} - \mathbf{Q}(\mathbf{Q}^T\mathbf{F}_I\mathbf{Q})^{-1}\mathbf{Q}^T\mathbf{F}_I \tag{9}$$

which transforms the FETI-H interface problem into:

$$\mathbf{P}^T\mathbf{F}_I\mathbf{P}\lambda \;=\; \mathbf{F}_I\mathbf{P}\lambda \;=\; \mathbf{P}^T\mathbf{d}\;; \tag{10}$$

$\mathbf{P}$ may be interpreted as a right preconditioner.

A suitable local preconditioning technique for the FETI-H algorithm

For FETI methods in general, it is also possible to derive another right preconditioner similar to the coarse projector $\mathbf{P}$, but instead of coming from a coarse space of optional admissible constraint, we approximate the interface problem using a local, subdomain based approximation.

The development of preconditioners for the traditional FETI method for elasticity problems can be presented in terms of mechanical arguments. In each iteration the FETI solver computes a "force" vector $\mathbf{p}^k$ and then the corresponding jump of the displacement across the interfaces. A simple way to accelerate convergence is then to invert this process, i.e., to impose the jump of the displacement field across the interface and compute the corresponding interface forces. These forces are then added back to $\mathbf{p}^k$ and the convergence is accelerated [FR94].

The implementation of such a preconditioner can be interpreted as follows. The forces on the interface are calculated by solving the following system (to simplify the notations we replace $\tilde{\mathbf{K}}$ by $\mathbf{K}$):

$$\begin{bmatrix} \mathbf{K}_{ii} & \mathbf{K}_{ib} \\ \mathbf{0} & \mathbf{I} \end{bmatrix} \begin{bmatrix} \widetilde{\mathbf{w}}_i^k \\ \{\widetilde{\mathbf{w}}_b^k\} \end{bmatrix} = \begin{bmatrix} \mathbf{0} \\ \mathbf{w}_b \end{bmatrix} \tag{11}$$

The solution is

$$\widetilde{\mathbf{w}}_i^k = -\mathbf{K}_{ii}^{-1}\mathbf{K}_{ib}\mathbf{w}_b \tag{12}$$

The subscripts i and b mean the internal and boundary d.o.f. and the brackets refers to known values. Now the corresponding interface force vector is:

$$\begin{bmatrix} \mathbf{K}_{ii} & \mathbf{K}_{ib} \\ \mathbf{K}_{ib}{}^T & \mathbf{K}_{bb} \end{bmatrix} \begin{bmatrix} \widetilde{\mathbf{w}}_i^k \\ \{\widetilde{\mathbf{w}}_b^k\} \end{bmatrix} = \begin{bmatrix} \mathbf{0} \\ \mathbf{K}_{bb}^{(s)} - \mathbf{K}_{ib}^{(s)\,T}\mathbf{K}_{ii}^{(s)\,-1}\mathbf{K}_{ib}^{(s)} \{\widetilde{\mathbf{w}}_b^k\} \end{bmatrix} \tag{13}$$

For a more efficient implementation of this preconditioner, we assemble the primal subdomain operator instead of approaching the inverse of the operator after assembling. This leads to the Dirichlet preconditioner:

$$\widetilde{\mathbf{F}_{\mathbf{I}}^{-1}}^{\mathbf{D}} = \sum_{s=1}^{s=N_s} \mathbf{B}^{(s)} \begin{bmatrix} \mathbf{0} & \mathbf{0} \\ \mathbf{0} & \mathbf{K}_{bb}^{(s)} - \mathbf{K}_{ib}^{(s)\,T}\mathbf{K}_{ii}^{(s)\,-1}\mathbf{K}_{ib}^{(s)} \end{bmatrix} \mathbf{B}^{(s)\,T} \tag{14}$$

The computation of the Dirichlet preconditioner needs an additional factorization of $\mathbf{K}_{ii}$, and storage. In each iteration, we also need one more forward/backward substitution. The following preconditioner,

$$\widetilde{\mathbf{F}_{\mathbf{I}}^{-1}}^{\mathbf{L}} = \sum_{s=1}^{s=N_s} \mathbf{B}^{(s)} \begin{bmatrix} \mathbf{0} & \mathbf{0} \\ \mathbf{0} & \mathbf{K}_{bb}^{(s)} \end{bmatrix} \mathbf{B}^{(s)\,T} \tag{15}$$

does not need any addtional storage or factorization. The idea of this *lumped* preconditioner is to lump all of the system matrix to the interface. From the mechanical point of view, for elasticity problems, it tries to find a set of lumped interface forces to reproduce the displacement jumps at the subdomains interface and only the interface nodes are allowed to displace.

For the Helmholtz problem, we intend to filter the vanishing modes by using the preconditioner, i.e., the modes that have a spatial frequency on the interface that is greater than the wavenumber of the global problem, i.e, to filter the eigenmodes associated with the eigenvalues that are close to zero. It has the drawback as it also changes the behavior of the other modes, in particular those of low frequency [dLBFM+98]. This process in the FETI-H method is reminiscent of the *lumped* preconditioner for elasticity problems, as our physical interpretation points out.

These considerations are logical and straightforward, but they do not consider the physical aspects of the Helmholtz problem, in particular the Sommerfeld condition. Furthermore, in the FETI-H method, we use a modified Lagrangian formulation that results in local interface matrices similar to the Sommerfeld condition contribution. The simplest idea to account for these facts is to incorporate into $\mathbf{K}_{bb}$ the contribution of the local interface matrices emanating from the modified Lagrangian. Then the lumped preconditioner is redefined as:

$$\widetilde{\mathbf{F}_{\mathbf{I}}^{-1}}^{\mathbf{L}} = \sum_{s=1}^{s=N_s} \mathbf{B}^{(s)} \begin{bmatrix} \mathbf{0} & \mathbf{0} \\ \mathbf{0} & \mathbf{K}_{bb}^{(s)} \pm ik\mathbf{M}_{bb}^{(s)} \end{bmatrix} \mathbf{B}^{(s)\,T} \tag{16}$$

REMARK: Note that the contribution $\mathbf{M}_{bb}^{(s)}$ incorporates into all of the interface of each subdomain is restricted by the "interface signing" compatibility constraint in [FML98a, FML+98b]. This may be interpreted not as a *Dirichlet* preconditioner, but as a *Dirichlet-Sommerfeld* preconditioner (at least locally). Although the numerical experiments in the next section show that this preconditioner improves convergence, it is still not clear if other definitions of this local *Dirichlet-Sommerfeld* preconditioner may provide a better option.

Numerical experiments

Table 1 The guided wave problem in 3D – $h = 1/36$, $ka = 10$, total size of the problem – 46656 dofs

N_θ	N_S	CR	CR*	BCG	BCG*	GCR	GCR*	GMRES	GMRES*
0	3×1	19	2	19	–	19	2	19	17
1	3×1	17	–	17	–	17	12	17	17
2	3×1	34	–	34	–	32	24	32	31
3	3×1	23	–	21	–	19	15	19	19
0	4×1	30	3	30	–	25	3	25	23
1	4×1	23	–	24	–	22	16	22	23
2	4×1	55	–	57	–	39	32	43	39
3	4×1	27	–	30	–	23	20	24	24
0	6×1	41	10	40	–	34	5	34	32
1	6×1	30	–	31	–	27	22	28	29
2	6×1	87	–	99	–	60	48	60	58
3	6×1	37	–	37	–	33	27	33	32
0	$2 \times 2 \times 2$	90	–	87	–	62	51	61	66
1	$2 \times 2 \times 2$	74	–	78	–	55	45	55	61
2	$2 \times 2 \times 2$	61	–	70	–	51	46	51	59
3	$2 \times 2 \times 2$	68	–	83	–	50	44	50	58
0	$3 \times 3 \times 3$	88	–	83	–	76	63	76	107
1	$3 \times 3 \times 3$	75	–	80	–	61	53	60	102
2	$3 \times 3 \times 3$	101	–	110	–	78	70	78	121
3	$3 \times 3 \times 3$	68	–	69	–	57	48	57	100
0	$4 \times 4 \times 4$	260	–	263	–	162	155	162	188
1	$4 \times 4 \times 4$	103	–	107	–	75	65	75	92
2	$4 \times 4 \times 4$	79	–	83	–	64	54	64	82
3	$4 \times 4 \times 4$	79	–	88	–	61	54	61	79
0	$6 \times 6 \times 6$	–	–	–	–	381	366	–	–
1	$6 \times 6 \times 6$	91	–	100	–	64	57	64	87
2	$6 \times 6 \times 6$	93	–	101	–	65	55	65	84
3	$6 \times 6 \times 6$	96	–	110	–	62	54	62	83

(*) indicates the algorithms with the local preconditioner and (–) stagnation

In this section we consider a 3D guided wave problem in a unit cube domain discretized using $36 \times 36 \times 36$ linear brick elements. Two opposite faces are subject to an unit Dirichlet b.c. and a Sommerfeld condition, respectively. All the other faces are subject to a homogeneous Neumann b.c.. The wave number for this problem is fixed to $ka = 10$ which gives almost 20 elements per wave length. The domain is decomposed into "slices" ($N \times 1$ subdomains) or cubes, i.e. $N \times N \times N$ subdomains. The results for this numerical experiment are given in Table 1 where we can assess the efficiency of the preconditioner and different algorithms. In this table, each column, corresponding to a solver, gives the number of iterations for the following convergence criteria: $||\mathbf{f} - [\mathbf{K} - k^2\mathbf{M}]\bar{\mathbf{u}}|| < 1e-6$, where $\bar{\mathbf{u}}$ is the solution resulting from the FETI-H iterative process. The same criteria was used for the results in Table 2.

Table 2 2D Submarine-shaped scatterer – SGI Origin 2000, 10 cpu's

GCR alg.	No Preconditioner	Preconditioner
Iterations	69	40
Total CPU Time	584.70	487.28
Preconditioning CPU Time	0.0	0.75

Comparing the different algorithms , the GCR algorithm has the best convergence properties and robustness, and, by using the preconditioner, we get good improvement in iteration count, for any mesh partition, as well as when combined with the coarse space. In contrast, the other algorithms do not get the same improvement as GCR and all of them stagnate when the preconditioner is combined with the coarse space or when a general mesh partition is used. For all these experiments, the residuals of the GCR algorithm are much smoother than those of all other algorithms, except for GMRES, which are similarly smooth. Also, it is important to note that the improvement of the preconditioner is worthwhile as it costs only about 0.15 % of the total solver cpu time, for a speed-up of the order of 15 %.

In table 2, we show the significant improvement observed for the FETI-H method by using the preconditioned GCR algorithm for an irregular mesh partition and decomposition in 2D. This is the case presented in [FML98a] and it concerns a submarine-shaped 2D scatterer with 1,077,432 nodes and 1,075,264 elements partitioned in 128 irregular subdomains.

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