Preconditioning of Iterative Eigenvalue Problem Solvers in Adaptive FETI-DP

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Abstract Adaptive FETI-DP and BDDC methods are robust methods that can be used for highly heterogeneous problems when standard approaches fail. In these approaches, local generalized eigenvalue problems are solved approximately, and the eigenvectors are used to enhance the coarse problem. Here, a few iterations of an approximate eigensolver are usually sufficient. Different preconditioning options for the iterative LOBPCG eigenvalue problem solver are considered. Numerical results are presented for linear elasticity problems with heterogeneous coefficients.

1 Introduction

Adaptive coarse spaces for FETI-DP or BDDC methods make use of locally computed (approximate) eigenvectors to enhance the coarse problem for faster Krylov convergence; for different approaches to domain decomposition methods with adaptive coarse spaces, see, e.g., [13, 5, 3, 17, 10, 6, 2, 14, 1, 15]. Of course, the solution of the corresponding local generalized eigenvalue problems in all these approaches adds a certain computational overhead to the setup of the method which then needs to be amortized in the iteration phase. It has been observed that an approximation of the eigenvectors already yields good convergence behavior; see [7]. In this paper, we consider different types of preconditioners for the iterative eigensolvers to obtain good approximate eigenvectors in a few steps.

We will give numerical results for the adaptive method of [8] for the equations of linear elasticity on a bounded polyhedral domain $\Omega \subset \mathbb{R}^3$, i.e., we search for $u \in \{v \in H^1(\Omega)^d : v = 0 \text{ on } \partial\Omega_D\}$ such that

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$$\int_\Omega 2\mu\varepsilon(u):\varepsilon(v)\mathrm{d}x+\int_\Omega \lambda\,\mathrm{div}(u)\mathrm{div}(v)\mathrm{d}x=\int_\Omega f\cdot v\mathrm{d}x+\int_{\partial\Omega_N} g\cdot v\mathrm{d}s. \qquad (1)$$

Here, $\partial\Omega_D\subset\partial\Omega$ is a subset with positive surface measure where Dirichlet boundary conditions are prescribed. Moreover, $\partial\Omega_N:=\partial\Omega\setminus\partial\Omega_D$ is the Neumann boundary, and λ,μ are the Lamé constants.

2 FETI-DP with a Generalized Transformation of Basis

For an introduction of FETI-DP; see, e.g., [4, 18]. Given a polyhedral domain $\Omega\subset\mathbb{R}^3$, we subdivide Ω into N nonoverlapping subdomains $\Omega_1,\dots,\Omega_N$ such that $\overline{\Omega}=\bigcup_{i=1}^N\overline{\Omega}_i$. The FETI-DP system is given by $F\lambda=d$, where

$$F=B_BK_{BB}^{-1}B_B^T+B_BK_{BB}^{-1}\widetilde{K}_{\Pi B}^T\widetilde{S}_{\Pi\Pi}^{-1}\widetilde{K}_{\Pi B}K_{BB}^{-1}B_B^T=B_\Gamma\widetilde{S}^{-1}B_\Gamma^T.$$

Here, $\widetilde{S}_{\Pi\Pi}$ constitutes the a priori coarse space where all vertex variables are chosen to be primal.

We then use the generalized transformation-of-basis approach, as presented in [9] and applied to the adaptive context in [8], to enforce additional, adaptively computed constraints, which we also denote as a posteriori constraints. The idea of the transformation-of-basis approach is to make a constraint vector c corresponding to a (generally local) constraint on the displacements u, i.e., $c^Tu=0$ an explicit basis vector and enforce the constraint by partial subassembly at the degree of freedom where the new basis vector is introduced. Given these (orthogonal) transformations $T^{(i)}$, $i=1,\dots,N$, we therefore solve systems with transformed stiffness matrices $\overline{K}^{(i)}=T^{(i)T}K^{(i)}T^{(i)}$, transformed displacements $\overline{u}^{(i)}=T^{(i)T}u^{(i)}$, and transformed right hand sides $\overline{f}^{(i)}=T^{(i)T}f^{(i)}$, $i=1,\dots,N$. In the standard approach, constraints in the jump operator B corresponding to these a posteriori primal constraints are removed. In the generalized approach, we do not remove these rows but assemble the a posteriori primal variables and directly redistribute the continuous values subsequently to all connected subdomains. That means, in contrast to the standard transformation-of-basis approach, we also allow for scalings of a posteriori primal variables, e.g., obtained from the adaptive approach in the next section. For more details, see [9, 8].

3 Adaptive FETI-DP with a Generalized Transformation of Basis

3.1 Generalized Local Eigenvalue Problems and Constraints for a Transformation of Basis

We now present briefly the adaptive approach introduced in [7, 8]. Given a domain decomposition $\overline{\Omega}=\bigcup_{i=1}^N\overline{\Omega}_i$, we define as an *edge* $\mathscr{E}^{il}$ the interior of $\partial\Omega_i\cap\partial\Omega_j\cap$

$\partial\Omega_l$, i.e., excluding the end points, and as a face $\mathscr{F}^{ij}$ the interior of $\partial\Omega_i \cap \partial\Omega_j$. Subsequently, we will use the index $s \in \{j,l\}$ to describe eigenvalue problems and their operators defined on faces ($s = j$) and edges ($s = l$), respectively. Let us note that eigenvalue problems on faces are defined on the closure of the face.

Let $\mathscr{Z}$ be either a face or an edge shared by two subdomains Ω_i and Ω_s. We introduce $B_{\overline{\mathscr{Z}}^{is}} = [B^{(i)}_{\overline{\mathscr{Z}}^{is}} B^{(s)}_{\overline{\mathscr{Z}}^{is}}]$ consisting of all the rows of $[B^{(i)}B^{(s)}]$ that contain exactly one $+1$ and one -1. Analogously, we introduce the scaled jump operator $B_{D,\overline{\mathscr{Z}}^{is}} = [B^{(i)}_{D,\overline{\mathscr{Z}}^{is}} B^{(s)}_{D,\overline{\mathscr{Z}}^{is}}]$ as the submatrix of $[B^{(i)}_D B^{(s)}_D]$. We need the local operators $S_{is} := \text{blockdiag}(S^{(i)}, S^{(s)})$ and $P_{D,\overline{\mathscr{Z}}^{is}} := B^T_{D,\overline{\mathscr{Z}}^{is}} B_{\overline{\mathscr{Z}}^{is}}$.

We now want to solve generalized eigenvalue problems on a subspace where S_{is} is positive definite since S_{is} is in general only semidefinite. We therefore study the problem of finding $w^k_{is} \in (\ker S_{is})^\perp$ with $\mu^k_{is} \geq \text{TOL}$, such that

$$s_{is}(P_{D,\overline{\mathscr{Z}}^{is}} v_{is}, P_{D,\overline{\mathscr{Z}}^{is}} w^k_{is}) = \mu^k_{is} s_{is}(v_{is}, w^k_{is}) \quad \forall v_{is} \in (\ker S_{is})^\perp. \tag{2}$$

There, $s_{is}(\cdot,\cdot) := (\cdot, S_{is}\cdot)$ for $u_{is} \times v_{is}$ with $u_{is}, v_{is} \in W_i \times W_s$ and W_i, W_s are the local finite element spaces on Ω_i and Ω_s. In practice, this is achieved by implementing projections Π_{is} and $\overline{\Pi}_{is}$ and making the computation numerically stable; cf. [13].

The constraint vectors $q^k_{is} := P^T_{D,\overline{\mathscr{Z}}^{is}} S_{is} P_{D,\overline{\mathscr{Z}}^{is}} w^k_{is}$ computed from the eigenvalue problems are either defined on edges or on closed faces. The constraints on closed faces are then split into (additional) edge constraints and constraints on the open face. This also enables an edge by edge and face by face orthogonalization.

In our approach, an edge constraint resulting from the eigenvalue problem of two subdomains sharing this edge will always be enforced for all subdomains sharing this edge. This does not increase the size of the coarse problem.

All the adaptive constraints are stored in an (orthogonalized) transformation matrix T which is block diagonal with respect to the subdomains and with respect to blocks corresponding to the faces and edges. The operator R^T performs the finite element assembly in the a posteriori primal variables, i.e., in all degrees of freedom which belong to an adaptively computed new basis vector. The transposed operator R then redistributes the values to the individual subdomains. We define the operator $R^T_\mu := (R^T R)^{-1} R^T$. For more details, see [9, 8].

In contrast to the standard transformation-of-basis approach, we use the same jump operator B as in the original FETI-DP master system. As a result, as in deflation, the preconditioned system has at least one zero eigenvalue for each adaptively computed constraint, i.e., for the a posteriori constraints.

The adaptive FETI-DP system using a generalized transformation of basis writes

$$\begin{aligned} \widehat{M}_T^{-1}\widehat{F}\lambda &:= (\widehat{B}_D \widehat{\widetilde{S}} \widehat{B}_D^T)\,(\widehat{\widetilde{S}}^{-1} \widehat{B}^T)\lambda \\ &:= (B_D T R_\mu (R^T T^T \widetilde{S} T R) R_\mu^T T^T B_D^T)(B T R (R^T T^T \widetilde{S} T R)^{-1} R^T T^T B^T)\lambda = d, \end{aligned} \tag{3}$$

where $\widehat{F}$ is the transformed FETI-DP operator and $\widehat{M}_T^{-1}$ is the transformed Dirichlet preconditioner. For this system, we now give, without proof, the condition number bound. For more details, see [8].

Theorem 1. *Let $N_{\mathscr{F}}$ denote the maximum number of faces of a subdomain, $N_{\mathscr{E}}$ the maximum number of edges of a subdomain, $M_{\mathscr{E}}$ the maximum multiplicity of an edge and* TOL *a given tolerance for solving the local generalized eigenvalue problems. If all vertices are chosen to be primal, the condition number $\kappa(\widehat{M}_T^{-1}\widehat{F})$ of the FETI-DP algorithm with adaptive constraints enforced by the generalized transformation-of-basis approach satisfies*

$$\kappa(\widehat{M}_T^{-1}\widehat{F}) \leq 4\max\{N_{\mathscr{F}}, N_{\mathscr{E}}M_{\mathscr{E}}\}^2\text{TOL}.$$

3.2 Solving the Local Generalized Eigenvalue Problems

Adaptive methods are most suitable for hard problems that are not solvable by standard techniques, e.g., as a result of strong heterogeneities present in the problem. However, as a result of these heterogeneities the local generalized eigenvalue problems can also be expected to be ill-conditioned, and unpreconditioned iterative eigensolvers may also struggle; see, e.g., [16]. As in [16], we use the iterative LOBPCG eigenvalue problem solver; see [12]. In practice, when using two projections Π_{is} and $\overline{\Pi}_{is}$ to remove the rigid body modes from S_{is}, the right hand side of the eigenvalue problems writes

$$\overline{\Pi}_{is}(\Pi_{is}S_{is}\Pi_{is} + \sigma_{is}(I-\Pi_{is}))\overline{\Pi}_{is} + \sigma_{is}(I-\overline{\Pi}_{is}) \tag{4}$$

where σ_{is} is chosen as $\sigma_{is} = \max(\text{diag}(S_{is}))$. The projection $I-\overline{\Pi}_{is}$ consists of the sum of several rank one matrices, and we usually avoid to building the matrix explicitly. The operator $\Pi_{is}S_{is}\Pi_{is} + \sigma_{is}(I-\Pi_{is})$ can be built cheaply by only scaling a few rows and columns of the Schur complements and adding some constants; see Figure 1 for the nonzero pattern of S_{is} and $\Pi_{is}S_{is}\Pi_{is} + \sigma_{is}(I-\Pi_{is})$.

We test five different preconditioners for the iterative eigensolver. First, we take a Cholesky decomposition of the fully assembled right hand side (4) as the (expensive) base line to compare against. We also test an LU and ILU(0) decomposition of $\Pi_{is}S_{is}\Pi_{is} + \sigma_{is}(I-\Pi_{is})$ and use the projection $\overline{\Pi}_{is}$ to remove the corresponding kernel from the preconditioner, i.e., we, e.g., use

$$\overline{\Pi}_{is}\mathbf{LU}\Big(\Pi_{is}S_{is}\Pi_{is} + \sigma_{is}(I-\Pi_{is})\Big)\overline{\Pi}_{is},$$

where $\mathbf{LU}(\cdot)$ denotes the computation of the LU decomposition of the argument. Finally, we also test two different local lumped versions, i.e., an LU and a ILU(0) decomposition of $K_{\Gamma\Gamma,is} = \text{blockdiag}(K_{\Gamma\Gamma}^{(i)}, K_{\Gamma\Gamma}^{(s)})$, so for the LU decomposition, we implement the preconditioner

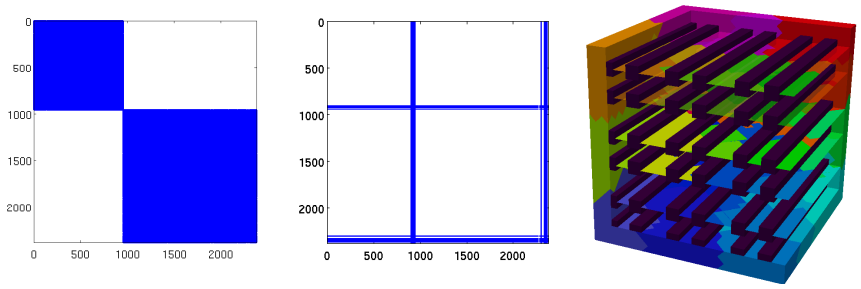

Fig. 1 Representative nonzero pattern of the matrices S_{is} (left) and $S_{is} - \left[\Pi_{is} S_{is} \Pi_{is} + \sigma_{is}(I - \Pi_{is})\right]$ (center) for two randomly chosen subdomains Ω_i, Ω_s. Composite material with irregular decomposition (right; visualization for $N = 27$ and $1/h = 10N^{1/3}$). In the right picture, large coefficients $\mathrm{E}_2 = 1e+06$ are shown in dark purple in the picture and low coefficients are not shown; subdomains are shown in different colors in the background and by half-transparent slices.

$$\overline{\Pi}_{is} \Pi_{is} \mathbf{LU}\Big(K_{\Gamma\Gamma,is}\Big) \Pi_{is} \overline{\Pi}_{is}.$$

3.3 Heuristic Modifications

As in [7], we will introduce two heuristic variants (denoted *Algorithm Ib* and *Ic*). The original algorithm is denoted *Algorithm Ia*.

Algorithm Ib: Reducing the number of edge eigenvalue problems We discard edge eigenvalue problems for edges that do not have high coefficient jumps in their neighborhood of one finite element.

Algorithm Ic: Reducing the number of edge constraints In addition, we also discard all edge constraints from face eigenvalue problems if there are no coefficient jumps in the neighborhood of the edge.

The condition number bound derived for *Algorithm Ia* will, in general, not hold for the two variants, however, it is likely that a modified theory, using slab techniques as in [10], can be derived for *Algorithm Ib*.

4 Numerical Results

We present numerical results for Algorithms Ia, Ib, and Ic. We have a soft matrix material with $\mathrm{E}_1 = 1$ with $4N^{2/3}$ stiff beams with $\mathrm{E}_2 = 1e+06$; see Fig. 1. We consider $\Omega = [0,1]^3$ with Dirichlet boundary conditions for the face with $x = 0$ and zero Neumann boundary conditions elsewhere; we have $f = [0.1, 0.1, 0.1]^T$ and $\mathrm{E}(x) \in \{1, 1e+6\}$. For the domain decomposition, the METIS graph partitioner

with options `-ncommon=3` and `-contig` is used. Each local eigenvalue problem is solved using LOBPCG with a block size 10, a given number of maximum iterations from $\{5, 25, 100\}$, and a preconditioner; see Section 3.2. Our a priori coarse space uses at least three primal vertices on each edge in order to remove local hinge modes; see [13, 7]. We also set edge nodes primal that belong to ~~an~~ single noded edges. The corresponding edge eigenvalue problem becomes superfluous. We assume the Young modulus $\mathrm{E}(x)$ to be constant on each finite element, and we use ρ-scaling in the form of patch-ρ-scaling. The coefficient $(\mathrm{E}(x^*))$ at a node x^* will be set as the maximum coefficient on the support of the corresponding nodal basis function φ_{x^*}; cf. [11]. In the tables, "κ" denotes the condition number of the adaptively preconditioned FETI-DP operator, "*its*" the number pcg iterations, "$|\Pi'|$" the size of the initial vertex coarse space and "$|\Pi|$" the size of the corresponding a posteriori coarse space; the number of subdomains is "N". The pcg algorithm is stopped after a relative reduction of the starting residual by 10^{-10} or when 500 iterations are reached.

5 Conclusion

We have presented results for different preconditioniers of the local generalized eigenvalue problems. Obviously, the most expensive algorithm, the Cholesky decomposition of the assembled right hand side of the eigenvalue problem yields the best results with respect to the condition numbers and the iteration counts of the FETI-DP algorithm. In this case, only a few iterations (e.g., 1-5) of the LOBPCG solver are sufficient; cf. also our results in [7, 8]. However, an LU or ILU(0)-factorization of $\Pi_{is} S_{is} \Pi_{is} + \sigma_{is}(I - \Pi_{is})$ with a few more iterations can suffice. To choose an LU or ILU decomposition of $\Pi_{is} S_{is} \Pi_{is} + \sigma_{is}(I - \Pi_{is})$ is a reasonable choice since this matrix can be built easily but just manipulating a few rows and columns of S_{is}; see Figure 1. Note that the slight differences in the condition numbers and iteration counts result from a small difference in the coarse space size. The results for the lumped preconditioner, an LU or ILU decomposition of $K_{\Gamma\Gamma,is}$ are given for completeness and to show that the results were not as satisfactory as expected. Eventually, note from [8] that also too many iterations (e.g., 200) of the local solver might not be helpful if the local scheme diverges without notice. A heuristic strategy for an (almost) optimal a priori choice of the maximum LOBPCG iteration number is still under development.

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Local Preconditioner: Chol$\left(\overline{\Pi}_{is}(\Pi_{is}S_{is}\Pi_{is}+\sigma_{is}(I-\Pi_{is}))\overline{\Pi}_{is}+\sigma_{is}(I-\overline{\Pi}_{is})\right)$.											
			Algorithm Ia			*Algorithm Ib*			*Algorithm Ic*		
N	$\lvert\Pi'\rvert$	LOBPCG max its	κ	its	$\lvert\Pi\rvert$	κ	its	$\lvert\Pi\rvert$	κ	its	$\lvert\Pi\rvert$
3^3	168	5	3.35	16	1905	3.35	16	1905	3.53	19	594
		25	8.89	18	2025	8.89	18	2025	9.12	21	684
		100	10.59	18	2013	10.59	18	2013	10.78	21	672
4^3	351	5	3.34	16	5259	3.34	16	5259	3.56	19	1674
		25	14.95	24	5535	14.95	24	5535	15.33	25	1869
		100	5.07	18	5496	5.07	18	5496	5.08	21	1848
Local Preconditioner: $\overline{\Pi}_{is}$**LU**$\left(\Pi_{is}S_{is}\Pi_{is}+\sigma_{is}(I-\Pi_{is})\right)\overline{\Pi}_{is}$.											
			Algorithm Ia			*Algorithm Ib*			*Algorithm Ic*		
N	$\lvert\Pi'\rvert$	LOBPCG max its	κ	its	$\lvert\Pi\rvert$	κ	its	$\lvert\Pi\rvert$	κ	its	$\lvert\Pi\rvert$
3^3	168	5	110.84	38	1872	110.84	38	1872	163.73	43	603
		25	3.84	18	1926	3.84	18	1926	3.84	20	660
		100	3.84	18	1938	3.84	18	1938	3.85	21	666
4^3	351	5	471.97	62	5074	471.97	62	5074	521.66	67	1647
		25	54.34	30	5259	54.34	30	5259	90.89	33	1830
		100	56.50	30	5328	56.50	30	5328	99.32	32	1884
Local Preconditioner: $\overline{\Pi}_{is}$**ILU(0)**$\left(\Pi_{is}S_{is}\Pi_{is}+\sigma_{is}(I-\Pi_{is})\right)\overline{\Pi}_{is}$.											
			Algorithm Ia			*Algorithm Ib*			*Algorithm Ic*		
N	$\lvert\Pi'\rvert$	LOBPCG max its	κ	its	$\lvert\Pi\rvert$	κ	its	$\lvert\Pi\rvert$	κ	its	$\lvert\Pi\rvert$
3^3	168	5	5.36	17	2088	5.36	17	2088	5.45	21	711
		25	3.82	20	1995	3.82	20	1995	3.84	21	678
		100	3.35	17	1998	3.35	17	1998	3.52	20	675
4^3	351	5	24.35	26	6225	24.35	26	6225	26.50	30	2394
		25	3.82	20	5964	3.82	20	5964	3.83	22	2277
		100	4.37	20	5850	4.37	20	5850	4.42	22	2181
Local Preconditioner: $\overline{\Pi}_{is}\Pi_{is}$**LU**$\left(K_{\Gamma\Gamma,is}\right)\Pi_{is}\overline{\Pi}_{is}$.											
			Algorithm Ia			*Algorithm Ib*			*Algorithm Ic*		
N	$\lvert\Pi'\rvert$	LOBPCG max its	κ	its	$\lvert\Pi\rvert$	κ	its	$\lvert\Pi\rvert$	κ	its	$\lvert\Pi\rvert$
3^3	168	5	1.81e+06	500	0	1.81e+06	500	0	1.81e+06	500	0
		25	3.83e+04	500	441	3.83e+04	500	441	1.56e+05	500	102
		100	452.95	126	442	452.95	126	442	468.46	129	81
4^3	351	5	1.06e+06	500	0	1.06e+06	500	0	1.06e+06	500	0
		25	5.97e+04	500	1254	5.97e+04	500	1254	1.72e+05	500	273
		100	677.56	181	936	677.56	181	936	685.30	183	213
Local Preconditioner: $\overline{\Pi}_{is}\Pi_{is}$**ILU(0)**$\left(K_{\Gamma\Gamma,is}\right)\Pi_{is}\overline{\Pi}_{is}$.											
			Algorithm Ia			*Algorithm Ib*			*Algorithm Ic*		
N	$\lvert\Pi'\rvert$	LOBPCG max its	κ	its	$\lvert\Pi\rvert$	κ	its	$\lvert\Pi\rvert$	κ	its	$\lvert\Pi\rvert$
3^3	168	5	1.81e+06	500	0	1.81e+06	500	0	1.81e+06	500	0
		25	3.26e+04	500	462	3.26e+04	500	462	8.40e+04	500	111
		100	197.47	108	324	197.47	108	324	200.09	110	75
4^3	351	5	1.06e+06	500	0	1.06e+06	500	0	1.06e+06	500	0
		25	4.56e+04	500	1236	4.56e+04	500	1236	8.51e+04	500	282
		100	2.54e+04	316	978	2.54e+04	316	978	6.15e+04	329	222

Table 1 Compressible linear elasticity on an irregular decomposition of $\overline{\Omega}=[0,1]^3$ with N subdomains, $1/h=10N^{1/3}$ and composite material with Young's modulus $\mathrm{E}_1=1$ and $\mathrm{E}_2=1e+06$. Coarse spaces for $\mathrm{TOL}=10$ for all generalized eigenvalue problems.

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