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Adaptive Coarse Spaces for FETI-DP in Three Dimensions with Applications to Heterogeneous Diffusion Problems

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1 Introduction

We consider an adaptive coarse space for FETI-DP or BDDC methods in three dimensions. We have user-given tolerances for certain eigenvalue problems which determine the computational overhead needed to obtain fast convergence. Similar adaptive strategies are available for many kinds of domain decomposition methods; see, e.g., Galvis and Efendiev [2010], Dolean et al. [2012], Spillane and Rixen [2013], Kim and Chung [2015], Klawonn et al. [2015], Mandel and Sousedík [2007], Dohrmann and Pechstein.

We will give numerical results for our algorithm for the diffusion equation on a bounded polyhedral domain Ω, i.e., for the weak formulation of

$$\begin{aligned} -\nabla\cdot(\rho\nabla u) &= f \quad \text{in } \Omega,\\ u &= 0 \quad \text{on } \partial\Omega_D,\\ \rho\nabla u\cdot\mathbf{n} &= 0 \quad \text{on } \partial\Omega_N. \end{aligned} \tag{1}$$

Here, $\partial\Omega_D \subset \partial\Omega$ is a subset with positive surface measure where Dirichlet boundary conditions are prescribed. Furthermore, $\partial\Omega_N := \partial\Omega \setminus \partial\Omega_D$ is the part of the boundary where Neumann boundary conditions are given and $\mathbf{n}$ is the outward pointing unit normal on $\partial\Omega_N$. The function $\rho = \rho(x)$ will be called coefficient (distribution).

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2 FETI-DP with Projector Preconditioning and Balancing

Due to space limitation, we will only provide the most important FETI-DP operators and the FETI-DP system. For a more detailed description of FETI-DP; see, e.g., Farhat et al. [2000], Toselli and Widlund [2005]. The FETI-DP system is given by $F\lambda = d$ where

$$F = B_B K_{BB}^{-1} B_B^T + B_B K_{BB}^{-1} \widetilde{K}_{\Pi B}^T \widetilde{S}_{\Pi\Pi}^{-1} \widetilde{K}_{\Pi B} K_{BB}^{-1} B_B^T,$$
$$d = B_B K_{BB}^{-1} f_B + B_B K_{BB}^{-1} \widetilde{K}_{\Pi B}^T \widetilde{S}_{\Pi\Pi}^{-1} \left(\left(\sum_{i=1}^{N} R_\Pi^{(i)T} f_\Pi^{(i)} \right) - \widetilde{K}_{\Pi B} K_{BB}^{-1} f_B \right).$$

Here, $\widetilde{S}_{\Pi\Pi}$ defines the primal coarse space which, in our case, will be given by all vertex variables being primal. We now present Projector Preconditioning and Balancing in a very short form; for a more detailed description see Klawonn and Rheinbach [2012], and for a semidefinite matrix F, Klawonn et al. [2016a]. Given a matrix U representing constraints $U^T B w = 0$, we define $P := U(U^T F U)^+ U^T F$ and solve the preconditioned system

$$M_{PP}^{-1} F\lambda := (I-P) M_D^{-1} (I-P)^T F\lambda = (I-P) M_D^{-1} (I-P)^T d.$$

Here, M_D^{-1} is the Dirichlet preconditioner. In our computations, we exclusively use patch-ρ-scaling (see Klawonn and Rheinbach [2007]) but other scalings are possible. We can also use the balancing preconditioner $M_{BP}^{-1} = M_{PP}^{-1} + U(U^T F U)^+ U^T$ instead of M_{PP}^{-1}.

3 Adaptive Constraints and Condition Number Bound

We now present our adaptive approach that is based on modifications of the approach in Mandel and Sousedík [2007]; see also Klawonn et al. [2016b] and Klawonn et al. [2016a]. In Klawonn et al. [2016b], for two dimensions, a complete theory including a condition number bound for the coarse space introduced by Mandel and Sousedík [2007] was given. However, this coarse space turns out not to be sufficient in three dimensions. In Klawonn et al. [2016a], we therefore have added certain edge eigenvalue problems to prove a condition number bound also in three dimensions and in the numerical experiments, we have focussed on elasticity. In the present paper, we consider scalar second-order elliptic problems.

For a given subdomain Ω_i, we assume that it shares an edge $\mathcal{E}$ and an adjacent face with Ω_j and Ω_k, respectively, while it only shares the edge $\mathcal{E}$ with Ω_l. More general cases can be treated analogously. In the following we will use the index $s \in \{j, l\}$ to describe simultaneously eigenvalue problems and their operators defined on faces ($s = j$) and edges ($s = l$), respectively. Note that eigenvalue problems on faces are defined on the closure of the face.

Let G be a face or an edge shared by Ω_i and Ω_s. Then, we define $B_{G_{is}} = [B^{(i)}_{G_{is}} B^{(s)}_{G_{is}}]$ as all the rows of $[B^{(i)} B^{(s)}]$ that contain exactly one $+1$ and one -1. In the same manner, we define the scaled matrix $B_{D,G_{is}} = [B^{(i)}_{D,G_{is}} B^{(s)}_{D,G_{is}}]$ as the submatrix of $[B^{(i)}_D B^{(s)}_D]$. Furthermore, define $S_{is} := \begin{pmatrix} S^{(i)} & 0 \\ 0 & S^{(s)} \end{pmatrix}$ and $P_{D_{is}} := B^T_{D,G_{is}} B_{G_{is}}$.

The space of functions in $W_i \times W_s$ that are continuous in the primal variables shared by Ω_i and Ω_s will be denoted by $\widetilde{W}_{is}$. Then, we introduce the ℓ_2-orthogonal projection Π_{is} from $W_i \times W_s$ to $\widetilde{W}_{is}$ as well as a second ℓ_2-orthogonal projection $\overline{\Pi}_{is}$ from $W_i \times W_s$ to $\mathrm{range}(\Pi_{is} S_{is} \Pi_{is} + \sigma(I - \Pi_{is}))$. There, σ is a possibly large positive constant, e.g., the maximum of the diagonal entries of S_{ij}, to avoid numerical instabilities. Without loss of generality we can asumme that the projections are symmetric.

Then, we build and solve the generalized eigenvalue problems

$$\begin{aligned} &\overline{\Pi}_{is} \Pi_{is} P^T_{D_{is}} S_{is} P_{D_{is}} \Pi_{is} \overline{\Pi}_{is} w^k_{is} \\ &= \mu^k_{is} (\overline{\Pi}_{is} (\Pi_{is} S_{is} \Pi_{is} + \sigma(I - \Pi_{is})) \overline{\Pi}_{is} + \sigma(I - \overline{\Pi}_{is})) w^k_{is}, \end{aligned} \tag{2}$$

for $\mu^k_{is} \geq$TOL. Let us note that the projections are built such that the right hand side of the eigenvalue problem (2) is symmetric positive definite; cf. Mandel and Sousedík [2007]. For an eigenvalue problem defined on (the closure of) a face (i.e. $s = j$), we split the computed constraint columns $u^k_{ij} := B_{D,G_{ij}} S_{ij} P_{D_{ij}} w^k_{ij}$ into several edge constraints $u^k_{ij,\mathcal{E}_m}$ and a constraint on the open face $u^k_{ij,\mathcal{F}}$, all extended by zero to the closure of the face. The splitting avoids coupling of the constraints and preserves a block structure of the constraint matrix; cf. Mandel et al. [2012]. We then enforce all the constraints

$$u^{k\,T}_{ij,\mathcal{E}_m} B_{F_{ij}} w_{ij} = 0,\ m = 1, 2, \ldots, \quad u^{k\,T}_{ij,\mathcal{F}} B_{F_{ij}} w_{ij} = 0.$$

For a given edge with corresponding edge eigenvalue problem, we enforce

$$w^{k\,T}_{il} P^T_{D_{il}} S_{il} P_{D_{il}} w_{il} = 0.$$

For $w \in W_i \times W_s$ satisfying the constraints, we have the local estimate

$$w^T_{is} \overline{\Pi}_{is} \Pi_{is} P^T_{D_{is}} S_{is} P_{D_{is}} \Pi_{is} \overline{\Pi}_{is} w_{is} \leq \mathrm{TOL}\, w^T_{is} \overline{\Pi}_{is} \Pi_{is} S_{is} \Pi_{is} \overline{\Pi}_{is} w_{is};$$

cf. Klawonn et al. [2016b]. For $w \in \widetilde{W}$ we have $\begin{pmatrix} R^{(i)} w \\ R^{(s)} w \end{pmatrix} \in \widetilde{W}_{is}$ and therefore $\Pi_{is} \begin{pmatrix} R^{(i)} w \\ R^{(s)} w \end{pmatrix} = \begin{pmatrix} R^{(i)} w \\ R^{(s)} w \end{pmatrix}$. As argued in Klawonn et al. [2016b] we have $\Pi_{is}(I - \overline{\Pi}_{is}) w_{is} = (I - \overline{\Pi}_{is}) w_{is}$. This gives $P_{D_{is}} \Pi_{is} (I - \overline{\Pi}_{is}) w_{is} = 0$ and

$S_{is}\Pi_{is}(I-\overline{\Pi}_{is})w_{is} = 0$. Therefore, for all $w_{is} \in \widetilde{W}_{is}$ with $w_{is}^{k\,T} P_{D_{is}}^T S_{is} P_{D_{is}} w_{is} = 0$, $\mu_{is}^k \geq \mathrm{TOL}$ we obtain

$$w_{is}^T \Pi_{is} P_{D_{is}}^T S_{is} P_{D_{is}} \Pi_{is} w_{is} \leq \mathrm{TOL} w_{is}^T \Pi_{is} S_{is} \Pi_{is} w_{is}; \tag{3}$$

cf. Mandel and Sousedík [2007].

Let $U = (u_1, \ldots, u_k)$ be the matrix where the adaptive constraints are stored in its columns. Then, $\widetilde{W}_U := \{w \in \widetilde{W} \,|\, U^T B w = 0\}$ will be the subspace of $\widetilde{W}$ which contains all elements $w \in \widetilde{W}$ satisfying the adaptively computed constraints, i.e., $Bw \in \ker U^T$. We are now ready to give the following lemma.

Lemma 1. *Let $N_{\mathcal{F}}$ denote the maximum number of faces of a subdomain, $N_{\mathcal{E}}$ the maximum number of edges of a subdomain, $M_{\mathcal{E}}$ 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, for $w \in \widetilde{W}_U$ it holds*

$$|P_D w|_{\widetilde{S}}^2 \leq 4 \max\{N_{\mathcal{F}}, N_{\mathcal{E}} M_{\mathcal{E}}\}^2 \mathrm{TOL} |w|_{\widetilde{S}}^2.$$

Proof. See Klawonn et al. [2016a].

We can now provide a condition number estimate for the preconditioned FETI-DP algorithm with all vertex constraints being primal and additional, adaptively chosen, edge and face constraints.

Theorem 1. *Let $N_{\mathcal{F}}$ denote the maximum number of faces of a subdomain, $N_{\mathcal{E}}$ the maximum number of edges of a subdomain, $M_{\mathcal{E}}$ 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 $\kappa(\widehat{M}^{-1}F)$ of the FETI-DP algorithm with adaptive constraints as described, e.g., enforced by the projector preconditioner $\widehat{M}^{-1} = M_{PP}^{-1}$ or the balancing preconditioner $\widehat{M}^{-1} = M_{BP}^{-1}$, satisfies*

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

Proof. See Klawonn et al. [2016a].

4 Heuristic Modifications

In this section we introduce two modifications of our algorithm. We will test the performance of the heuristically reduced coarse spaces along with the algorithm presented before.

Reducing the number of edge eigenvalue problems Our first modification consists of discarding edge eigenvalue problems on edges where no coefficient jumps occur. Therefore, we traverse the corresponding edge nodes and check for coefficient jumps. If no jumps occur we will not solve the corresponding edge eigenvalue problem and discard it with all possible constraints. Let us note that the condition number bound mentioned before might no longer hold if we use this strategy. However, due to slab techniques, see, e.g., Klawonn et al. [2015], the condition number is expected to stay bounded independently of the coefficients.

Reducing the number of edge constraints The second approach uses the strategy discussed before and discards additionally edge constraints from face eigenvalue problems, if there are no coefficient jumps in the neighborhood of the edge.

5 Numerical Results

In this section, we will give numerical results for five different algorithms. First, we will present results for our new algorithm that is covered by theory (denoted by '*Alg. Ia*') and two modifications thereof; see also Klawonn et al. [2016a] where these algorithms were introduced for elasticity. By '*Alg. Ib*' we will denote the modification using only the first strategy presented in Sect. 4. We will also test a variant using both heuristics of Sect. 4. This algorithm will be denoted '*Alg. Ic*'. The performance of these algorithms will be compared to the approaches of Mandel et al. [2012]. By '*Alg. III*' we denote the 'classic' approach which discards all edge constraints from face eigenvalue problems. The coarse space enriched by those edge constraints but without edge constraints from edge eigenvalue problems will be denoted by '*Alg. II*'.

For all algorithms we will start with an extended first coarse space. Given the coarse space consisting of primal vertices, we will add some additional edge nodes. We will set those edge nodes primal that belong to an edge eigenvalue problem on a short edge, i.e., an edge with only one dual node. Then, the corresponding edge eigenvalue problem will become superfluous.

We use a singular value decomposition with a drop tolerance of $1e-6$ to orthogonalize all adaptively computed constraints. We use the balancing preconditioner to enforce the resulting constraints. For simplicity, we assume $\rho(x)$ to be constant on each finite element and we use ρ-scaling in the form of patch-ρ-scaling. The coefficient at a node will be set as the maximum coefficient on the support of the corresponding nodal basis function; cf. Klawonn and Rheinbach [2007]. In the experiments, we use an irregular partitioning of the domain using the METIS graph partitioner with options `-ncommon=3` and `-contig`. Let us note that Alg. III might be sufficient if regular decompositions are chosen and jumps only appear at subdomain faces; see Mandel et al. [2012]. We will therefore just test irregular decompositions.

In all tables, "κ" denotes the condition number of the preconditioned FETI-DP operator, "*its*" is the number of iterations of the pcg algorithm

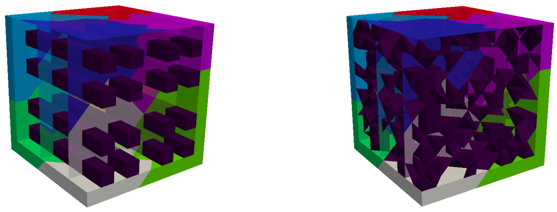

Fig. 1 Composite material (left) and randomly distributed coefficients (right) with irregular decomposition. High coefficients $E_2 = 1e+06$ are shown in dark purple in the picture; low coefficients are not shown. Subdomains are shown in different colors in the background and by half-transparent slices. Visualization for $N = 8$ and $H/h = 5$.

and "$|U|$" denotes the size of the corresponding second coarse space. By "N" we denote the number of subdomains. For our modified coarse space, we also give the number of edge eigenvalue problem as "$\#\mathcal{E}_{ewp}$" and in parentheses the percentage of these in the total number of eigenvalue problems. Our stopping criterion for the pcg algorithm is a relative reduction of the starting residual by 10^{-10}, and the maximum number of iterations is set to 500. The condition numbers κ, which we report in the tables, are estimates from the Krylov process. We will consider $\Omega = [0, 1]^3$, discretized by a structured fine mesh of cubes, each containing five tetrahedra. We apply Dirichlet boundary conditions for the face with $x = 0$ and zero Neumann boundary conditions elsewhere. Moreover, let $f = 0.1$ and $\rho(x) \in \{1, 1e+6\}$.

A composite material We consider a soft matrix material with $E = 1$ and stiff inclusions in the form of $4N^{2/3}$ beams with $E = 1e+06$; see Fig. 1. In Table 1, we see that Alg. III always leads to high condition numbers and even to nonconvergence ($its = 500$) in three of four cases. The use of edge constraints from face eigenvalue problems (cf. Alg. II) can neither guarantee small condition numbers but results in convergence within a maximum of about 90 iterations. Although only Alg. Ia is covered by our theoretical bound, Alg. Ia, Ib, and Ic can guarantee condition numbers around the size of the prescribed tolerance and convergence within 30-40 iterations. Here, Alg. Ic gives the best performance: it uses the smallest coarse space and leads to convergence in a small number of iterations.

Let us note that the number of edge eigenvalue problems here is larger than in the case of linear elasticity (cf. Klawonn et al. [2016a]). This is due to the fact that, in case of elasticity, we have to select additional primal vertices to remove hinge modes on curved edges. Then, edge eigenvalue problems on certain short edges become superfluous. Since this is not necessary for the diffusion equation, and since it also enlarges the primal coarse space, we do not carry this out here and accept a higher number of eigenvalue problems.

Random coefficients We now perform 100 runs using randomly generated coefficients (20% high and 80% low) for different numbers of subdo-

Composite material, irregular partitioning and $H/h = 5$											
		Alg. Ia, Ib, and Ic				*Alg. II*			*Alg. III*		
N		κ	its	$\lvert U\rvert$	$\mathcal{E}_{evp}$	κ	its	$\lvert U\rvert$	κ	its	$\lvert U\rvert$
4^3	a)	9.54	36	1784	41 (14.9%)	9.78	37	1765	2.23e+06	500	609
	b)	9.78	36	1783	30 (11.3%)						
	c)	10.68	39	1475	30 (11.3%)						
6^3	a)	11.72	38	6455	166 (15.1%)	5.13e+05	98	6364	3.13e+06	500	2057
	b)	11.72	38	6455	134 (12.6%)						
	c)	11.72	39	5701	134 (12.6%)						
8^3	a)	12.34	39	15292	390 (14.1%)	2.27e+05	62	15120	2.99e+06	500	4921
	b)	12.34	39	15292	334 (12.4%)						
	c)	12.34	40	13682	334 (12.4%)						

Table 1 Compressible linear elasticity with $E_1 = 1$, $E_2 = 1e + 06$. Coarse spaces for TOL $= 10$ for all generalized eigenvalue problems.

Randomly distributed coefficients, irregular partitioning, and $H/h = 5$.												
			Alg. Ia, Ib, and Ic				*Alg. II*			*Alg. III*		
N			κ	its	$\lvert U\rvert$	$\#\mathcal{E}_{evp}$	κ	its	$\lvert U\rvert$	κ	its	$\lvert U\rvert$
4^3	$\overline{x}$	a)	8.81	30.64	1913.92	41 (14.9%)	3.92e+05	43.61	1889.83	2.62e+06	500	675.53
		b)	8.81	30.64	1913.92	41 (14.9%)						
		c)	8.81	30.64	1913.72	41 (14.9%)						
	$\widetilde{x}$	a)	8.76	31	1918	41 (14.9%)	2.31e+05	42.5	1893.5	2.57e+06	500	676
		b)	8.76	31	1918	41 (14.9%)						
		c)	8.76	31	1918	41 (14.9%)						
	σ	a)	0.88	1.32	43.57	-	5.12e+05	10.41	43.25	7.42e+05	0	22.05
		b)	0.88	1.32	43.57	-						
		c)	0.88	1.32	43.67	-						
5^3	$\overline{x}$	a)	9.26	32.19	3992.86	61 (10.3%)	2.29e+05	55.35	3954.5	2.96e+06	500	1357.53
		b)	9.26	32.19	3992.86	61 (10.3%)						
		c)	9.26	32.19	3992.55	61 (10.3%)						
	$\widetilde{x}$	a)	9.20	32	3997.5	61 (10.3%)	2.01e+05	52.5	3955.5	2.79e+06	500	1359.5
		b)	9.20	32	3997.5	61 (10.3%)						
		c)	9.20	32	3996	61 (10.3%)						
	σ	a)	0.86	0.88	69.31	-	2.09e+05	15.05	68.58	7.52e+05	0	33.67
		b)	0.86	0.88	69.31	-						
		c)	0.86	0.90	69.38	-						

Table 2 Compressible linear elasticity with $E_1 = 1$, $E_2 = 1e + 06$. Coarse spaces for TOL $= 10$ for all generalized eigenvalue problems.

mains; see Table 2. For $N \in \{4^3, 5^3\}$, we see that the classical Alg. III does not converge in any single run and always leads to a condition number of at least $1e + 05$. Although Alg. II converges in all cases it exhibits a condition number of $1e + 05$ or higher in 71 ($N = 4^3$) and 73 ($N = 5^3$) runs. The performance of Alg. Ia, Ib, and Ic is almost identical. For these algorithms, the condition number is always lower than 15, and convergence is reached within 35 iterations.

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