Adaptive Coarse Space Selection in the BDDC and the FETI-DP Iterative Substructuring Methods: Optimal Face Degrees of Freedom

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Summary. We propose adaptive selection of the coarse space of the BDDC and FETI-DP iterative substructuring methods by adding coarse degrees of freedom (dofs) on faces between substructures constructed using eigenvectors associated with the faces. Provably the minimal number of coarse dofs on the faces is added to decrease the condition number estimate under a target value specified a priori. It is assumed that corner dofs are already sufficient to prevent relative rigid body motions of any two substructures with a common face. It is shown numerically on a 2D elasticity problem that the condition number estimate based on faces is quite indicative of the actual condition number and that the method can select adaptively a hard part of the problem and concentrate computational work there to achieve the target value for the condition number and good convergence of the iterations, at a modest cost.

1 Introduction

The BDDC and FETI-DP methods are iterative substructuring methods that use coarse degrees of freedom associated with corners and edges (in 2D) or faces (in 3D, further on just faces) between substructures, and they are currently the most advanced versions of the BDD and FETI families of methods. The BDDC method by Dohrmann [2] is a Neumann-Neumann method of Schwarz type [3]. The BDDC method iterates on the system of primal variables reduced to the interfaces between the substructures and it can be understood as further development of the BDD method by Mandel [11]. The FETI-DP method by Farhat et al. [5, 4] is a dual method that iterates on a system for Lagrange multipliers that enforce continuity on the interfaces,

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and it is a further development of the FETI method by Farhat and Roux [6]. Algebraic relations between FETI and BDD methods were pointed out by Rixen et al. [13], Klawonn and Widlund [8], and Fragakis and Papadrakakis [7]. A common bound on the condition number of both the FETI and the BDD method in terms of a single inequality in was given by [8]. In the case of corner constraints only, methods same as BDDC were derived as primal versions of FETI-DP by Cros [1] and Fragakis and Papadrakakis [7], who have also observed that the eigenvalues of BDD and a certain version of FETI are identical. Mandel, Dohrmann, and Tezaur [12] have proved that the eigenvalues of BDDC and FETI-DP are identical and they have obtained a simplifed and fully algebraic version (i.e., with no undetermined constants) of a common condition number estimate for BDDC and FETI-DP, similar to the estimate by Klawon and Widlund [8] for BDD and FETI.

In this contribution, we show how to use the algebraic estimate from [12] to develop an adaptive fast method. This estimate makes it possible to compute the condition number bound from the matrices in the method as the solution of an eigenvalue problem. By restricting the eigenproblems onto pairs of adjacent substructures with a common face, we obtain a reliable heuristic estimate of the condition number based on eigenvalues associated with the faces. Finally, we show how to use the eigenvectors to obtain coarse degrees of freedom that result in an optimal decrease of the condition number estimate. We show on numerical examples that the condition number estimates are quite tight and such adaptive approach can result in the concentration of computational work in a small troublesome part of the problem, which leads to good convergence behavior at a small added cost.

Related work on adaptive adaptive coarse space selection has focused on the global problem of selecting the smallest number of corners to prevent coarse mechanisms (Lesoinne [10]) and the smallest number of (more general) coarse degrees of freedom to assure asymptotically optimal convergence estimates (Klawonn and Widlund [9]). In contrast, our estimates are local in nature and we assume that corner degrees of freedom are already sufficient to prevent relative rigid body motions of any two substructures with a common face.

2 Formulation of BDDC and FETI-DP

We need to briefly recall the formulation of the methods and the condition number bound. Let K_i be the stiffness matrix and v_i the vector of degrees of freedom (dofs) for substructure i. We want to solve the problem in decomposed form

$$\frac{1}{2}v^T K v - v^T f \to \min, \quad v = \begin{bmatrix} v_1 \\ \vdots \\ v_N \end{bmatrix} \quad K = \begin{bmatrix} K_1 & & \\ & \ddots & \\ & & K_N \end{bmatrix}$$

subject to continuity dofs between substructures. Partitioning the dofs in each subdomain i into internal and interface (boundary)

$$K_i = \begin{bmatrix} K_i^{ii} & K_i^{ib} \\ K_i^{ib\,T} & K_i^{bb} \end{bmatrix}, \quad v_i = \begin{bmatrix} v_i^i \\ v_i^b \end{bmatrix}, \quad f_i = \begin{bmatrix} f_i^i \\ f_i^b \end{bmatrix},$$

and eliminating the interior dofs we obtain the problem reduced to interfaces

$$\frac{1}{2} w^T S w - w^T g \to \min, \quad S = \mathrm{diag}(S_i), \quad S_i = K_i^{bb} - K_i^{ib^T} K_i^{ii-1} K_i^{ib},$$

again subject to continuity of dofs between substructures

In BDD type methods, the continuity of dofs between substructures is enforced by imposing common values on substructures interfaces: $w = Ru$ for some u, where

$$R = \begin{bmatrix} R_1 \\ \vdots \\ R_N \end{bmatrix}$$

and R_i is the operator of restriction of global dofs on the interfaces to substructure i. In FETI type methods, continuity of dofs between substructures is enforced by the constraint $Bw = 0$, where the entries of B are typically $0, \pm 1$. By construction, we have $R_i R_i^T = I$ and range $R = \mathrm{null} B$.

A BDDC or FETI-DP method is specified by the choice of coarse dofs and the choice of weights for intersubdomain averaging. To define the coarse problem for BDDC, choose a matrix Q_P^T that selects coarse dofs u_c from global interface dofs u, e.g. as values at corners or averages on sides:

$$u_c = Q_P^T u.$$

We define $\widetilde{W}$ as the space of all vectors of substructure interface dofs that are continuous between substructures,

$$\widetilde{W} = \{ w \in W : \exists u_c \forall i : C_i w_i = R_{ci} u_c \}$$

where $C_i = R_{ci} Q_P^T R_i^T$, and R_{ci} restricts a vector of all coarse dof values into a vector of coarse dof values that can be nonzero on substructure i . The dual approach in FETI-DP is to construct Q_D such that $\widetilde{W} = \mathrm{null}\, Q_D^T B$.

In BDDC, the intersubdomain averaging is defined by the matrices $D_P = \mathrm{diag}\,(D_{Pi})$ that form a decomposition of unity, $R^T D_P R = I$. The corresponding dual matrices in FETI-DP are are $B_D = [D_{D1} B_1, \ldots D_{DN} B_N]$, where the dual weights D_{Di} are defined so that $B_D^T B + R R^T D_P = I$.

The BDDC method is then the method of conjugate gradients for the assembled system $Au = R^T g$ with the system matrix $A = R^T S R$ and the preconditioner P defined by $Pr = R^T D_P\,(\Psi u_c + z)$, where u_c is the solution of the coarse problem $\Psi^T S \Psi u_c = \Psi^T D_P^T R r$ and z is the solution of

$$\begin{array}{ll} Sz + C^T\mu = D_P^T Rr \\ Cz \qquad = \quad 0 \end{array},$$

which is a collection of independent substructure problems. The coarse basis functions Ψ are defined by energy minimization,

$$\begin{bmatrix} S & C^T \\ C & 0 \end{bmatrix} \begin{bmatrix} \Psi \\ \Lambda \end{bmatrix} = \begin{bmatrix} 0 \\ R_c \end{bmatrix}.$$

The FETI-DP method solves the saddle point problem

$$\min_{w \in \widetilde{W}} \max_{\lambda} \mathcal{L}(w, \lambda) = \max_{\lambda} \min_{w \in \widetilde{W}} \mathcal{L}(w, \lambda),$$

where $\mathcal{L}(w, \lambda) = \frac{1}{2} w^T S w - w^T f + w^T B^T \lambda$ by iterating on the dual problem $\frac{\partial \mathcal{F}(\lambda)}{\partial \lambda} = F\lambda - h = 0$, where

$$\mathcal{F}(\lambda) = \min_{w \in \widetilde{W}} \mathcal{L}(w, \lambda),$$

by conjugate gradients with the preconditioner $M = B_D S B_D^T$. See [12] for more details.

3 Condition Number Estimates

Theorem 1 ([12]). *The eigenvalues of the preconditioned operators PA of BDDC and MF of FETI-DP are same except for eigenvalues of zero and one, and the condition numbers satisfy*

$$\kappa_{\text{BDDC}} = \kappa_{\text{FETI-DP}} \leq \omega = \sup_{w \in \widetilde{W}} \frac{\left\| B_D^T B w \right\|_S^2}{\left\| w \right\|_S^2} = \sup_{w \in \widetilde{W}} \frac{\left\| R R^T D_P w \right\|_S^2}{\left\| w \right\|_S^2}.$$

Here, the condition number is the ratio of the largest and the smallest nonzero eigenvalue. Zero eigenvalues in FETI-DP are caused by redundant constraints, common in practice.

We estimate the condition number bound as the maximum of the bounds from Theorem 1 computed for the problem restricted to a pair of adjacent substructures i, j with a common face:

$$\omega \approx \widetilde{\omega} = \max_{ij} \omega_{ij}, \quad \omega_{ij} = \sup_{w_{ij} \in \widetilde{W}_{ij}} J_{ij}\left(w_{ij}\right), \tag{1}$$

where J_{ij} is the Rayleigh quotient

$$J_{ij}\left(w_{ij}\right) = \frac{w_{ij}^T B_{ij}^T B_{Dij} S_{ij} B_{Dij}^T B_{ij} w_{ij}}{w_{ij}^T S_{ij} w_{ij}},$$

and the subscript $_{ij}$ means restriction on the pair of substructures i and j.

Theorem 2. *Let $a > 0$, Π_{ij} be the orthogonal projection onto $\widetilde{W}_{ij}$, and $\overline{\Pi}_{ij}$ be the orthogonal projection onto the complement of*

$$\operatorname{null}\left(Z_{ij}^T \left[\Pi_{ij} S_{ij} \Pi_{ij} + a\left(I - \Pi_{ij}\right)\right] Z_{ij}\right),$$

where

$$\operatorname{null} S_i \subset \operatorname{range} Z_i, \quad \operatorname{null} S_j \subset \operatorname{range} Z_j, \quad Z_{ij} = \begin{bmatrix} Z_i \\ Z_j \end{bmatrix}.$$

Then the stationary values $\omega_{ij,1} \geq \omega_{ij,2} \geq \ldots$ and the corresponding stationary vectors $w_{ij,k}$ of the Rayleigh quotient J_{ij} on $\widetilde{W}_{ij}$ satisfy

$$X_{ij} w_{ij,k} = \omega_{ij,k} Y_{ij} w_{ij,k} \tag{2}$$

with Y_{ij} positive definite, where

$$\begin{aligned} X_{ij} &= \Pi_{ij} B_{ij}^T B_{Dij} S_{ij} B_{Dij}^T B_{ij} \Pi_{ij}, \\ Y_{ij} &= \left(\overline{\Pi}_{ij}\left(\Pi_{ij} S_{ij} \Pi_{ij} + a\left(I - \Pi_{ij}\right)\right) \overline{\Pi}_{ij} + a\left(I - \overline{\Pi}_{ij}\right)\right) \end{aligned}$$

The coarse basis functions Ψ_i can be used as Z_i because the span of coarse basis functions contains rigid body modes, but rigid body modes are often available directly, which leads to a more efficient computation.

4 Optimal Coarse Degrees of Freedom on Faces

Writing $\widetilde{W}_{ij}$ in the dual form $\widetilde{W}_{ij} = \operatorname{null} Q_{Dij}^T B_{ij}$ suggests how to add coarse dofs in an optimal way to decrease the estimate $\widetilde{\omega}$.

Theorem 3. *Suppose $\ell_{ij} \geq 0$ and the dual coarse dof selection matrix Q_{Dij}^T is augmented to become $\left[Q_{Dij}^T, q_{Dij,1}^T, \ldots, q_{Dij,\ell_{ij}}^T\right]$ with $q_{Dij,k}^T = w_{ij,k}^T B_{ij}^T B_{Dij} S_{ij} B_{Dij}^T$, where $w_{ij,k}^T$ are the eigenvectors from (2). Then $\omega_{ij} = \omega_{ij,\ell_{ij}+1}$, and $\omega_{ij} \geq \omega_{ij,\ell_{ij}+1}$ for any other augmentation of Q_{Dij}^T by at most ℓ_{ij} columns.*

In particular, if $\omega_{ij,\ell_{ij}+1} \leq \tau$ for all pairs of substructures i, j with a common face, then $\widetilde{\omega} \leq \tau$.

Theorem 3 allows to gurantee that the condition number estimate $\widetilde{\omega} \leq \tau$ for a given target value τ, by adding the smallest possible number of face coarse dofs.

The primal coarse space selection mechanism that corresponds to this augmentation can be seen easily in the case when the entries of B_{ij} are $+1$ for substructure i and -1 for substructrure j. Then $w_{ij} \in \widetilde{W}_{ij}$ can be written as

$$Q_{Dij}^T (I_{ij} w_i - I_{ji} w_j) = 0$$

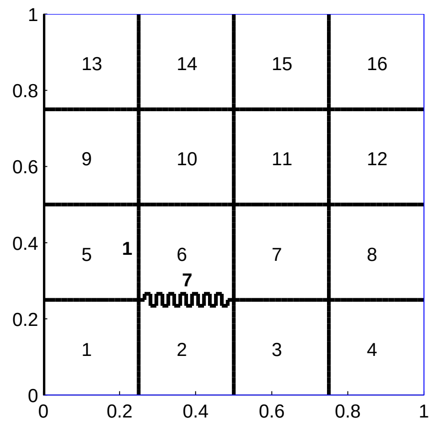

Fig. 1. Mesh with $H/h = 16$, 4×4 substructures, and one jagged edge between substructures 2 and 6. Zero displacement is imposed on the left edge. For compressible elasticity (Tables 1 and 2(a)) and tolerance $\tau = 10$, 7 coarse dofs at the jagged edge and 1 coarse dof at an adjacent edge are added automatically.

where I_{ij} is the $0-1$ matrix that selects from w_i the degrees of freedom on the intersection of the substructures i and j. Each column of q_D of Q_{Dij} defines a coarse degree of freedom associated with the interface of substructures i and j. The corresponding column q_P of Q_P is such that

$$q_P^T R_i^T = q_D^T I_{ij} \tag{3}$$

Because R_i is also a $0-1$ matrix, this means that the vector q_P is formed by a scattering of the entries of the vector q_D.

5 Numerical results

Consider plane elasticity discretized by bilinear elements on a rectangular mesh decomposed into 16 substructure, with one edge between substructures jagged (Fig. 1). The eigenvalues $\omega_{ij,k}$ associated with edges between substructures (Table 1) clearly distinguish between the problematic edge and the others. Adding the coarse dofs created from the associated eigenvectors according to Theorem 3 decreases the condition number estimate $\widetilde{\omega}$ and improves convergence at the cost of increasing the number of coarse dofs. This effect is even more pronounced for almost incompressible elasticity where the iterations converge poorly or not at all without the additional coarse dofs. This incompressible elasticity problem is particularly hard for an iterative method because standard bilinear elements were used instead of stable elements or reduced integration. In all cases, the condition number estimate $\widetilde{\omega}$ is quite close to the actually observed condition number κ (Table 2).

i	j	$\omega_{ij,1}$	$\omega_{ij,2}$	$\omega_{ij,3}$	$\omega_{ij,4}$	$\omega_{ij,5}$	$\omega_{ij,6}$	$\omega_{ij,7}$	$\omega_{ij,8}$
1	2	3.7	2.3	1.4	1.3	1.1	1.1	1.1	1.1
1	5	5.8	3.2	2.3	1.4	1.2	1.1	1.1	1.1
2	3	6.0	2.5	1.7	1.3	1.2	1.1	1.	1.1
2	6	21.7	19.5	17.8	14.9	14.5	11.7	11.2	9.7
3	4	3.3	2.3	1.4	1.3	1.1	1.1	1.1	1.1
3	7	7.1	5.1	3.2	1.8	1.4	1.3	1.2	1.1
4	8	5.9	3.4	2.6	1.4	1.2	1.1	1.1	1.1
5	6	12.0	4.9	4.4	1.8	1.6	1.3	1.3	1.2
5	9	5.9	3.4	2.6	1.4	1.3	1.3	1.1	1.1
6	7	8.7	4.9	3.9	1.8	1.5	1.3	1.2	1.1
6	10	7.3	4.8	3.4	1.8	1.4	1.3	1.2	1.1

Table 1. Several largest eigenvalues $\omega_{ij,k}$ for several edges for the elasticity problem from Fig. 1 with $H/h = 16$. $(i, j) = (2, 6)$ is the jagged edge.

H/h	$Ndof$	τ	Nc	$\widetilde{\omega}$	κ	it
4	578		42	10.3	5.6	19
		10	43	5.2	4.0	18
		3	44	3.0	4.0	18
		2	58	2.0	2.8	15
16	8450		42	22	20	37
		10	50	8.7	9.9	29
		3	77	3.0	4.6	22
		2	112	2.0	2.6	15
64	132098		42	87	40	55
		10	89	9.8	9.9	36
		3	151	3.0	4.7	22
		2	174	2.0	2.9	17

(a) compressible elasticity

H/h	$Ndof$	τ	Nc	$\widetilde{\omega}$	κ	it
4	578		42	285	208	64
		10	68	8.0	8.6	28
		3	89	2.9	4.6	22
		2	114	2.0	2.6	16
16	8450		42	1012	1010	161
		10	87	9.8	9.9	29
		3	77	3.0	4.6	22
		2	126	2.0	2.9	19
64	132098		42	6910	NA	∞
		10	183	9.8	9.7	37
		3	213	3.0	4.9	26
		2	274	2.0	3.0	20

(b) almost incompressible

Table 2. BDDC results for plane elasticity on a square with one jagged edge. The Lamé coefficients are $\lambda = 1$ and $\mu = 2$ for (a), and $\lambda = 1000$ and $\mu = 2$ for (b). H/h is the number of elements per substructure in one direction, $Ndof$ the number of dofs in the problem, τ the condition number tolerance as in Theorem 3, Nc the number of coarse dofs, $\widetilde{\omega}$ the apriori condition number estimate from (1), κ the approximate condition number computed from the Lanczos sequence in conjugate gradients, and it the number of BDDC iterations for relative residual tolerance 10^{-8}.

References

1. J.-M. Cros. A preconditioner for the Schur complement domain decomposition method. In Ismael Herrera, David E. Keyes, and Olof B. Widlund, editors, *Domain decomposition methods in science and engineering*, pages 373–380. National Autonomous University of Mexico (UNAM), México, 2003. Papers from the 14th International Conference on Domain Decomposition Methods held at the Universidad Nacional Autónoma de México, Cocoyoc, January 6–12, 2002.

2. Clark R. Dohrmann. A preconditioner for substructuring based on constrained energy minimization. *SIAM J. Sci. Comput.*, 25(1):246–258, 2003.
3. Maksymilian Dryja and Olof B. Widlund. Schwarz methods of Neumann-Neumann type for three-dimensional elliptic finite element problems. *Comm. Pure Appl. Math.*, 48(2):121–155, 1995.
4. Charbel Farhat, Michael Lesoinne, and Kendall Pierson. A scalable dual-primal domain decomposition method. *Numerical Linear Algebra with Applications*, 7:687–714, 2000. Preconditioning techniques for large sparse matrix problems in industrial applications (Minneapolis, MN, 1999).
5. Charbel Farhat, Michel Lesoinne, Patrick LeTallec, Kendall Pierson, and Daniel Rixen. FETI-DP: a dual-primal unified FETI method. I. A faster alternative to the two-level FETI method. *International Journal for Numerical Methods in Engineering*, 50(7):1523–1544, 2001.
6. Charbel Farhat and Francois-Xavier Roux. A Method of Finite Element Tearing and Interconnecting and its Parallel Solution Algorithm. *Internat. J. Numer. Methods Engrg.*, 32:1205–1227, 1991.
7. Yannis Fragakis and Manolis Papadrakakis. The mosaic of high performance domain decomposition methods for structural mechanics: Formulation, interrelation and numerical efficiency of primal and dual methods. *Comput. Methods Appl. Mech. Engrg.*, 192:3799–3830, 2003.
8. Axel Klawonn and Olof B. Widlund. FETI and Neumann-Neumann iterative substructuring methods: connections and new results. *Comm. Pure Appl. Math.*, 54(1):57–90, 2001.
9. Axel Klawonn and Olof B. Widlund. Selecting constraints in dual-primal FETI methods for elasticity in three dimensions. In R. Kornhuber, R. Hoppe, J. Priaux, O. Pironneau, O. Widlund, and J. Xu, editors, *Domain Decomposition Methods in Science and Engineering*, Lecture Notes in Computational Science and Engineering, pages 67–81. Springer, 2004. Proceedings of the 15th International Conference on Domain Decomposition Methods in Berlin, Germany, 2003.
10. M. Lesoinne. A FETI-DP corner selection algorithm for three-dimensional problems. pages 217–223. National Autonomous University of Mexico (UNAM), México, 2003. Papers from the 14th International Conference on Domain Decomposition Methods held at the Universidad Nacional Autónoma de México, Cocoyoc, January 6–12, 2002.
11. Jan Mandel. Balancing domain decomposition. *Comm. Numer. Methods Engrg.*, 9(3):233–241, 1993.
12. Jan Mandel, Clark R. Dohrmann, and Radek Tezaur. An algebraic theory for primal and dual substructuring methods by constraints. Appl. Numer. Math., in print. Available online October 2004, http://dx.doi.org/10.1016/j.apnum.2004.09.022 Proceedings of the 6th IMACS International Symposium on Iterative Methods, Denver, CO, March 2003.
13. Daniel J. Rixen, Charbel Farhat, Radek Tezaur, and Jan Mandel. Theoretical comparison of the FETI and algebraically partitioned FETI methods, and performance comparisons with a direct sparse solver. *Int. J. Numer. Meth. Engrg*, 46:501–534, 1999.