Adaptive Coarse Space Selection in
BDDC and FETI-DP Iterative Substructuring Methods:
Towards Fast and Robust Solvers

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Synopsis


2. Numerical computation of the condition number bound from a global eigenvalue problem: *in experiments, reasonably sharp*

3. Estimate of the condition number bound from local (face based) eigenvalue problems: *in experiments, reasonably accurate*

4. Optimal selection of face averages from local eigenvectors to decrease the condition number estimate $\Rightarrow$

   *practical and efficient adaptive algorithm*
The FETI-DP and BDDC Methods

- Both the BDDC and FETI-DP methods are build from same components. The methods use different algebraic algorithms.


- **BDDC (Dohrmann 2002):** method from the Balancing Domain Decomposition (BDD) family (Mandel 1993), based on Additive Schwarz framework of Neumann Neumann type (Dryja, Widlund 1995); convergence analysis Mandel and Dohrmann 2002. For corner constraints only, Cros 2003.

- The eigenvalues of the preconditioned operators of FETI-DP and BDDC are identical (Mandel, Dohrmann, Tezaur 2004)
Development of Adaptive FETI-DP and BDDC Algorithms

- **Continue algebraic analysis as long as possible** before switching to calculus (FEM, functional analysis) arguments, abstract from a specific FEM framework to widen the scope of the methods.

- **Algebraic bounds on the condition number** allow to select components of the methods adaptively.

- **Select method components adaptively to force condition number estimate under a specified value:** control number of iterations but each iteration gets more expensive. Future: minimize estimated total computational work.
Substructuring and Reduction to Interfaces

$K_i$ is the stiffness matrix for substructure $i$, symmetric positive problem in decomposed form

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

+ continuity of dofs between substructures
partition the dofs in each subdomain $i$ into internal and interface (boundary)
and eliminate interior dofs

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

$\Rightarrow$ decomposed problem reduced to interfaces

$$\frac{1}{2} w^T S w - w^T g \rightarrow \min, \quad S = \text{diag}(S_i), \quad S_i = K_{bb}^{bb} - K_{ib}^{ibT} K_{ii}^{ii} - 1 K_{ib}^{ib}$$

+continuity of dofs between substructures
Enforcing Intersubdomain Continuity

**primal methods (BDD,N-N):**

$U$ is the space of global dofs

$R_i : U \to W_i$ restriction to substructure $i$, $R = \begin{bmatrix} R_1 \\ \vdots \\ R_N \end{bmatrix}$

continuity of dofs between substructures: $w = Ru$ for some $u \in U$

**dual methods (FETI):**

continuity of dofs between substructures: $Bw = 0$

$B = [B_1, \ldots, B_N] = \begin{bmatrix} 1 & -1 & 0 & \cdots \\ \vdots & \vdots & \vdots & \ddots \end{bmatrix} : W \to \Lambda$

by construction:

$R_i R_i^T = I$, \quad \text{range } R = \text{null } B$
Choose matrix $Q_T^P$ that selects coarse dofs: $u_c = Q_T^P u$ (e.g. values of global dofs $u$ at corners, averages on sides)

Define $R_{ci}$: all constraint values $\mapsto$ values that can be nonzero on substructure $i$, define $C_i = R_{ci}Q_T^P R_i^T$:

\[
    u_c = 0 \iff C_i w_i = 0 \quad \forall \ i
\]

Assume the generalized coarse dofs define interpolation:

$\forall w \in U \exists u_c \forall i : C_i R_i w = R_{ci} u_c$

$\iff$ a coarse dof can only involve nodes adjacent to the same set of substructures

Define subspace of vectors with coarse dofs continuous across substructures:

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

Dual approach (FETI): construct $Q_D$ so that

$w \in \tilde{W} \iff Q_D^T B w = 0$
Intersubdomain Averaging and Weight matrices

primary diagonal weight matrices $D_{Pi} : W_i \rightarrow W_i$, $D_P = \text{diag}(D_{Pi})$

decomposition of unity: $R^T D_P R = I$

purpose: average between subdomains to get global dofs: $u = R^T D_P w$

dual weight matrices $D_{Di} : \Lambda \rightarrow \Lambda$, defined by $d^\alpha_{ij} = d^\alpha_j$

- $d^\alpha_j$: diagonal entry of $D_{Pj}$ associated with the same global dof $\alpha$
- $d^\alpha_{ij}$: diagonal entry of $D_{Di}$ for $\Omega_i$ and $\Omega_j$ and the same global dof $\alpha$

define $B_D = [D_{D1}B_1, \ldots D_{DN}B_N]$, then

$B_D^T$ is a generalized inverse of $B$: $BB_D^T B = B$

associated projections are complementary: $B_D^T B + RR^T D_P = I$


same identities hold also for other versions of the operators
FETI-DP Approach

enforce equality of coarse dofs directly: \( Q^T_D B w = 0 \)
enforce the rest of the constraints \( B w = 0 \) (or all) by multipliers \( \lambda \)

\[ \implies \text{saddle point problem: } \min_{w \in \tilde{W}} \max_{\lambda} \mathcal{L}(w, \lambda) = \max_{\lambda} \min_{w \in \tilde{W}} \mathcal{L}(w, \lambda) \]

\[ \mathcal{L}(w, \lambda) = \frac{1}{2} w^T S w - w^T f + w^T B^T \lambda \]

\[ \tilde{W} = \left\{ w : Q^T B w = 0 \right\} \text{ functions with coarse dofs same between substructures} \]

\[ \implies \text{dual problem: } \frac{\partial \mathcal{F}(\lambda)}{\partial \lambda} = 0, \quad \mathcal{F}(\lambda) = \min_{w \in \tilde{W}} \mathcal{L}(w, \lambda) \]

preconditioner \( M = B_D S B_D^T \)

\( Q^T_D B w = 0 \) enforces continuity
- of values across crosspoints (Farhat, Lesoinne, Le Tallec, Pierson, Rixen 2001)
BDDC: Balancing Domain Decomposition Based on Constraints

The system operator of the BDDC method is the assembled Schur complement

\[ A = R^T S R. \]

The preconditioner \( P \) is defined by

\[ Pr = R^T D_P (\Psi u_c + z) \]

where \( u_c \) is the solution of SPD coarse problems

\[ \Psi^T S \Psi u_c = \Psi^T D_P^T Rr \]

and \( z \) is the solution of

\[ S z + C^T \mu = D_P^T Rr \]
\[ C z = 0 \]

(independent substructure problems because of block structure of \( S \) and \( C \))

Here, the coarse basis functions \( \Psi \) are defined by energy minimization

\[ \begin{bmatrix} S & C^T \\ C & 0 \end{bmatrix} \begin{bmatrix} \Psi \\ \Lambda \end{bmatrix} = \begin{bmatrix} 0 \\ R_c \end{bmatrix}. \]
Assume that $S$ is positive definite on $\tilde{W}$: there is enough constraints to eliminate mechanisms between substructures in the whole model.

Theorem.

$$
\kappa_{\text{BDDC}} = \kappa_{\text{FETI-DP}} \leq \omega = \sup_{w \in \tilde{W}} \frac{\| B^T D B w \|^2_S}{\| w \|^2_S}
$$

Theorem. Eigenvalues or the preconditioned operator are the same except for zero eigenvalue in FETI-DP and different multiplicity of eigenvalue one.

Zero eigenvalues of FETI-DP are from redundant constraints in $B$. All other eigenvalues are $\geq 1$. 

Algebraic Bound on Condition Number
Related Work: Theoretical Asymptotic Condition Number Bounds

The algebraic bound + standard substructuring arguments (Klawonn, Widlund, Dryja 2002) \(\implies \omega \leq C \left(1 + \log^2 \frac{H}{h}\right)\)

However, the arguments are quite subtle, especially for elasticity.

A similar asymptotic bound (with \(h, H\) independent constants) in terms of \(B^T_D B\) was given by Klawonn and Widlund 2001 for some other versions of FETI and BDD.

We carry on our algebra a bit longer so our algebraic bound here has no undetermined constants. It also helps that the analysis is simpler in the case of FETI-DP and BDDC.

This introduction was all taken from Mandel, Dohrmann, Tezaur 2004. The following material is new.
Lemma. If $\Pi$ is an orthogonal projection, $a \neq 0$, and $\omega \neq 0$, then

$$\Pi T \Pi u = \omega \Pi S \Pi u \land u \in \text{range } \Pi \iff \Pi T \Pi u = \omega (\Pi S \Pi + a (I - \Pi)) u$$

Theorem. $\forall a > 0$,

$$\kappa_{\text{BDDC}} = \kappa_{\text{FETI-DP}} \leq \omega = \sup_{w \in \tilde{W}} \frac{\|B_D^T B w\|_S^2}{\|w\|_S^2} = \sup_{w} \frac{w^T \Pi B_T^T B_D S B_T^T B \Pi w}{w^T (\Pi S \Pi + a (I - \Pi)) w}$$

where $w^T (\Pi S \Pi + a (I - \Pi)) w > 0$ and $\Pi$ is the orthogonal projection onto $\tilde{W}$:

$$\Pi = I - \begin{bmatrix} C^T & 0 \end{bmatrix} \begin{bmatrix} C C^T & R_c \\ R_c^T & 0 \end{bmatrix}^{-1} \begin{bmatrix} C \\ 0 \end{bmatrix}$$

Approximate max eigenvalue and eigenvector can be computed easily e.g. by LOBPCG (Knyazev, 2001). Or just run the iterations and compute the extreme eigenvalues from the Lanczos sequence generated by PCG.
Heuristic Local Condition Number Estimates

We estimate the convergence bound by the maximum of the same bounds computed from two adjacent substructures $i, j$ at a time:

$$w_{ij} = \begin{bmatrix} w_i \\ w_j \end{bmatrix}, \quad S_{ij} = \begin{bmatrix} S_i & 0 \\ 0 & S_j \end{bmatrix}, \quad C_{ij} = \begin{bmatrix} C_i & 0 \\ 0 & C_j \end{bmatrix}$$

etc. Define $B_{ij}$ as the submatrix of $[B_i \ B_j]$ consisting of all rows that have exactly one $+1$ and one $-1$, define $\tilde{W}_{ij}$ accordingly. We propose

$$\omega \approx \tilde{\omega} = \max_{ij} \omega_{ij}$$

where

$$\omega_{ij} = \sup_{w_{ij} \in \tilde{W}_{ij}} \frac{\left\| B_{ij} w_{ij} \right\|_{S_{ij}}^2}{\left\| w_{ij} \right\|_{S_{ij}}^2} = \sup_{w_{ij} \in \tilde{W}_{ij}} \frac{w_{ij}^T B_{ij} S_{ij} w_{ij}}{w_{ij}^T S_{ij} w_{ij}}$$

We assume that there is already enough constraints between the two substructures to eliminate mechanisms (i.e., relative motion).
Computation of Local Condition Number Estimates

We have restricted all computations on two substructures $i$ and $j$ with a common face and assumed that there is already enough constraints to eliminate relative motion between the two substructures.

Theorem.

$$
\omega_{ij} = \sup_{w_{ij}} \frac{w_{ij}^T \Pi_{ij} B_{ij}^T B_{Dij} S_{ij} B_{Dij}^T B_{ij} \Pi_{ij} w_{ij}}{w_{ij}^T \left[ \Pi_{ij} S_{ij} \Pi_{ij} + a \left( I - \Pi_{ij} \right) \right] w_{ij}}
$$

Problem: both matrices are still typically singular because of rigid body modes that move substructures $i$ and $j$ as a whole. This makes computing the eigenvalues harder. Need to add to the right hand side matrix a projection on the complement of the nullspace of $\left[ \Pi_{ij} S_{ij} \Pi_{ij} + a \left( I - \Pi_{ij} \right) \right]$. 
Find matrices $Z_i, Z_j$ that generate a superspace of rigid body modes of the two substructures:

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

(the coarse basis functions may be used, $Z_i = \Psi_i$ because span of coarse basis functions contains rigid body modes, but there are too many of them; RBM often available directly)

construct generators of nullspace by solving a smaller eigenvalue problem

$$\text{range } Q = \text{null} \left( \Pi_{ij} S_{ij} \Pi_{ij} + a \left( I - \Pi_{ij} \right) \right)$$

$$= \text{null} \left( Z_{ij}^T \left[ \Pi_{ij} S_{ij} \Pi_{ij} + a \left( I - \Pi_{ij} \right) \right] Z_{ij} \right)$$
Computation of Local Condition Number Estimates (cont.)

Theorem.

\[ \omega_{ij} = \sup_{w_{ij}} \frac{w_{ij}^T X_{ij} w_{ij}}{w_{ij}^T Y_{ij} w_{ij}} \]

where

\[ X_{ij} = \Pi_{ij} B_{ij}^T B_{Dij} S_{ij} B_{Dij}^T B_{ij} \Pi_{ij}, \]

\[ Y_{ij} = \left( \Pi_{ij} \left( \Pi_{ij} S_{ij} \Pi_{ij} + a \left( I - \Pi_{ij} \right) \right) \Pi_{ij} + a \left( I - \Pi_{ij} \right) \right) > 0 \]

and \( \Pi_{ij} = \left( I - QQ^T \right) \) is the orthogonal projection onto range \( \left( \Pi_{ij} S_{ij} \Pi_{ij} + a \left( I - \Pi_{ij} \right) \right) \).

This is a symmetric generalized matrix eigenvalue problem with one of the matrices positive definite, easy to solve.
Optimal Constraints to Decrease the Rayleigh Quotient

The condition number estimate is the maximum of Rayleigh quotient over space $\tilde{W}_{ij}$. We can add constraints to make $\tilde{W}_{ij}$ smaller.

**Lemma** (well known) Let $X$, $Y$ be symmetric positive semidefinite operators in $n$-dimensional space $V$, $Y$ positive definite, and

$$X u_k = \lambda_k Y u_k, \quad \lambda_1 \geq \lambda_2 \geq \ldots \geq \lambda_n$$

all eigenvalues and eigenvectors. Then for any $V_k \subset V$ such that dim $V_k = k$,

$$\max \{ J(u) : \langle v, Xu \rangle = 0, \forall v \in V_k \} \geq \lambda_{k+1}$$

with equality if and only if

$$V_k = \text{span} \{ u_1, \ldots, u_k \}$$

$k$ constraints from eigenvectors eliminates the $k$ largest eigenvalues

This will allow us to add constraints that decrease the estimates $\omega_{ij}$ optimally.
Correspondence Between Dual and Primal Definitions of Coarse DOFs

Dual view: \( \tilde{W}_{ij} = \{w_{ij} : Q^T_{Di} B_{ij} w_{ij} = 0\} \) is the space defined by averages of continuity constraints: \( w_{ij} \) orthogonal to something

Primal view: \( w_{ij} \in \tilde{W}_{ij} \iff \) the values of the coarse dofs \( q_P R^T_i w_i \) are same for both substructures

Entries of \( B_{ij} \) are +1 for \( i \) and −1 for \( j \) \( \Rightarrow \) the value of the coarse dof is the common value on both sides: \( B_{ij} w_{ij} = I_{ij}w_i - I_{ji}w_j \) (\( I_{ij} \) selects from \( w_i \) the DOFs on interface between substructures \( i \) and \( j \))

\[
\begin{align*}
\tilde{W}_{ij} & \cong Q^T_{Di} I_{ij} w_i = Q^T_{Di} I_{ji} w_j \\
\end{align*}
\]

Each column of \( q_D \) of \( Q_{Di} \) defines a coarse degree of freedom which can be written using the corresponding column \( q_P \) of \( Q_P \) as

\[
q^T_P R^T_i w_i = q^T_D I_{ij} w_i
\]

\( R_i \) and \( I_{ij} \) are 0-1 \( \Rightarrow q_P \) is a scattering of the entries of the \( q_D \).
Construction of Optimal Additional Face Constraints

Recall that $\omega_{ij}$ is the maximal eigenvalue $\lambda_{ij,k}$ of

$$B^{T}_{ij}B_{Di}S_{ij}B^{T}_{Dij}B_{ij}u_{ij,k} = \lambda_{ij,k}S_{ij}u_{ij,k}$$

Given target $\tau$ add columns $q_D$ of $Q_D$ so that

$$\underbrace{u^{T}_{ij,k}B^{T}_{ij}B_{Di}S_{ij}B^{T}_{Dij}}_{q^{T}_{D}} B_{ij}w_{ij} = 0 \quad \forall \lambda_{ij,k} > \tau$$

$\implies$ guaranteed that the heuristic condition estimate $\omega_{ij} \leq \tau$

The additional (primal) coarse degrees of freedom are then defined by

$$q^{T}_{P}R^{T}_{i}w_{i} = q^{T}_{D}I_{ij}w_{i}$$
Adaptive Coarse DOFs for Plane Elasticity
\( \lambda = 1 \mu = 2 \)

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Ndof: number of degrees of freedom
\( \tau \) condition number target: coarse dofs added for all \( \lambda_{ij} > \tau \); corners only if not specified
\( \tilde{\omega} = \max \omega_{ij} \): heuristic condition estimate
\( \kappa \) approximate condition number estimate from PCG
it: number of iterations for stopping tolerance \( 10^{-8} \)
Adaptive Constraints for $H/h = 16$

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Number of added constraints $\tau = 10$

Number of substructures:

1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16
Adaptive Coarse DOFs for Almost Incompressible Elasticity

\[ \lambda = 1000 \quad \mu = 2 \]

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Ndof: number of degrees of freedom
\( \tau \): condition number target: coarse dofs added for all \( \lambda_{ij} > \tau \); corners only if not specified
\( \tilde{\omega} \): heuristic condition estimate
\( \kappa \): approximate condition number estimate from PCG
it: number of iterations for stopping tolerance \( 10^{-8} \)
Related Work: Selection of Constraints for Elasticity

Lesoinne 2001: selection of corner constraints to prevent global mechanisms (= guarantee that $S$ is positive definite on $\tilde{W}$). Examples that $S$ positive definite on $\{u : Cu = 0\}$ (each substructure sufficiently constrained by coarse dofs to prevent rigid body modes) is not enough.

Klawonn, Widlund, 2004: how to select a minimal number of corner constraints to prevent global mechanisms and to get rigorous $C \left(1 + \log^2 \frac{H}{h}\right)$ condition number bounds.

Here we assume that $S$ is positive definite on $\tilde{W}$ and even more: there is already enough constraints to prevent mechanism between any two substructures with a common face.

Dohrmann 2004: additional constraint (flux) for almost incompressible elasticity; Jing Li 2002: edge average constraints on all velocity components for Stokes problem. Here we find the additional constraints automatically.
Conclusion

Demonstrated that condition number is estimated accurately and reliably

Developed efficient control of condition number by additional constraints: a robust method

Shown that additional constraints concentrated on the problem spot: low computational complexity

Works also for almost incompressible elasticity.

No other information needed besides the matrix in substructure form and what are the corners.

Applicable to both FETI-DP and BDDC.

Future: tests and development on real problems; adaptive algorithms to minimize total work