An Algebraic Convergence Theory for Primal and Dual Substructuring Methods by Constraints

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The methods

- FETI-DP (Farhat, Lesoinne, Pierson 2000): substructuring method of the FETI family (Farhat, Roux, 1992) , based on Lagrange Multipliers,

- BDDC (Dohrmann 2002): method from the Balancing Domain Decomposition family (Mandel 1993), based on Additive Schwarz framework of Neumann Neumann type (Dryja, Widlund 1995)

- both methods for SPD problems from structural mechanics, implemented in the SALINAS code at Sandia, massively parallel

Objectives

- Algebraic bounds on the condition number to select components of the methods adaptively (future)

- 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

Components of the methods

$$\mathbf{FETI-DP} \Longleftarrow \left\{ \begin{array}{c} \textbf{Substructuring and reduction to interfaces} \\ \textbf{Enforcing intersubdomain continuity} \\ \textbf{Intersubdomain averaging and weight matrices} \\ \textbf{Augmented constraints and coarse dofs} \end{array} \right\} \Longrightarrow \mathbf{BDDC}$$

Both the BDDC and FETI-DP methods are build from similar components.
For a comparison, all components of both methods need to be identical.
The methods then use basically different algebraic algorithms.

Substructuring and reduction to interfaces

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

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

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

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

$\Longrightarrow$ decomposed problem reduced to interfaces

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

$+$continuity of dofs between substructures

Enforcing intersubdomain continuity

dual methods (FETI):

continuity of dofs between substructures: $Bw = 0$

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

primal methods (BDD,...):

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 $u \in U$

easy to see:

$$R_i R_i^T = I, \quad \text{range}\, R = \text{null}\, B$$

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 $d_{ij}^{\alpha} = d_j^{\alpha}$
- d_j^{α}: diagonal entry of D_{Pj} associated with the same global dof α
- d_{ij}^{α}: diagonal entry of D_{Di} for Ω_i and Ω_j and the same global dof α

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: $B_D^T B + RR^T D_P = I$

Rixen, Farhat, Tezaur, Mandel 1998, Rixen, Farhat 1999, Klawonn, Widlund, Dryja 2001, 2002, Fragakis, Papadrakakis 2003
same identities hold also for other versions of the operators

Augmented constraints and coarse dofs

Choose matrix Q_P^T that selects coarse dofs: $u_c = Q_P^T w$ (e.g. values at corners, averages on sides)

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

$$u_c = 0 \iff C_i w_i = 0 \ \forall \ i$$

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

FETI constraints $Bw = 0$ augmented by $Q_D^T Bw = 0$ so that

$$w \in \widetilde{W} \Leftrightarrow Q_D^T Bw = 0$$

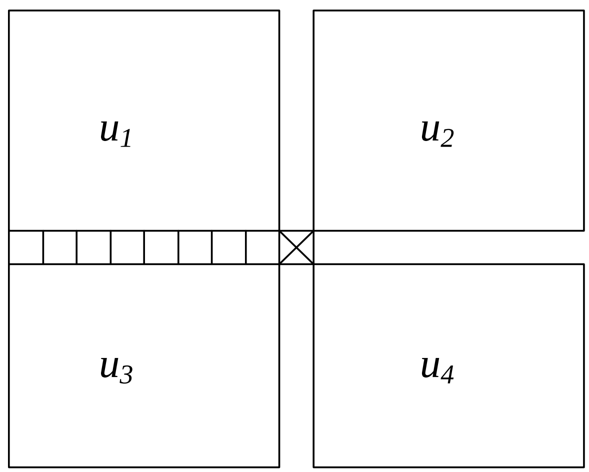
FETI Approach

$$w \in W = W_1 \times \ldots \times W_N, \quad S = \begin{bmatrix} S_1 & & \\ & \ddots & \\ & & S_N \end{bmatrix}$$

Continuity constraints between substructures: $Bw = 0$

$$B = [B_1, \ldots, B_N] = \begin{bmatrix} 1 & -1 & 0 & \ldots \\ \vdots & \vdots & \vdots & \vdots \end{bmatrix}$$

Problem: $\mathcal{E}(w) = \frac{1}{2} w^T S w - w^T g \to$ min subject to $Bw = 0$
Enforce constraints by Lagrange multipliers λ, eliminate w, solve problem for λ by PCG: solving independent problems with S_i, possibly singular



FETI-DP Approach

$$\left.\begin{array}{c}\text{enforce selected constraints directly : } Q_D^T B w = 0 \\ \text{enforce the rest of the constraints } Bw = 0 \text{ (or all) by multipliers } \lambda\end{array}\right\}$$

$\Longrightarrow$ saddle point problem: $\displaystyle\min_{w \in \widetilde{W}} \max_{\lambda} \mathcal{L}(w,\lambda) = \max_{\lambda} \min_{w \in \widetilde{W}} \mathcal{L}(w,\lambda)$

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

$\widetilde{W} = \left\{ w : Q^T B w = 0 \right\}$ functions that satisfy the augmenting constraints

$\Longrightarrow$ dual problem: $\frac{\partial \mathcal{F}(\lambda)}{\partial \lambda} = 0, \quad \mathcal{F}(\lambda) = \displaystyle\min_{w \in \widetilde{W}} \mathcal{L}(w,\lambda)$

preconditioner $M = B_D S B_D^T$

$Q_D^T B w = 0$ enforces continuity

- of values across crosspoints (Farhat, Lesoinne, Le Tallec, Pierson, Rixen 2001)
- also of averages across edges and faces (for 3D) (Farhat, Lesoinne, Pierson 2000, Pierson thesis 2000, Klawonn, Widlund, Dryja 2002)

Original FETI-DP Implementation

Farhat, Lesoinne, Pierson 2000:

$w = w_c + w_r$, w_c values on corners, w_r is "remainding dofs"

$$\left.\begin{array}{c}\text{same values on corners as new common variables } w_c : w_{i,c} = R_{i,c} u_c \\ \text{enforce the same averages across the edges by new multiplier } \mu\end{array}\right\}$$

$\Longrightarrow$ local problems: eliminate w_r $\Longrightarrow$ coarse problem: eliminate u_c and μ $\Longrightarrow$ dual problem

$$\mathcal{F}(\lambda) = \min_{u_c} \max_{\mu} \min_{w_r} \left(\mathcal{E}(R_c u_c + w_r, \lambda) + (R_c u_c + w_r)^T B^T Q_D \mu \right) \to \max$$

coarse problem for u_c, μ from $\min \max$ $\Longrightarrow$ indefinite, sparse

Alternative FETI-DP Setting

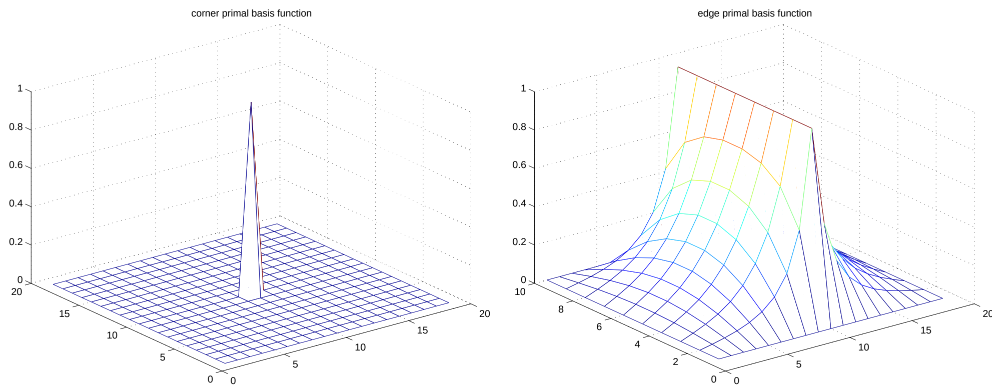
Klawonn, Widlund, Dryja 2002:

$$\widetilde{W} \;=\; \widetilde{W}_{\Pi} \oplus \widetilde{W}_{\Delta}$$

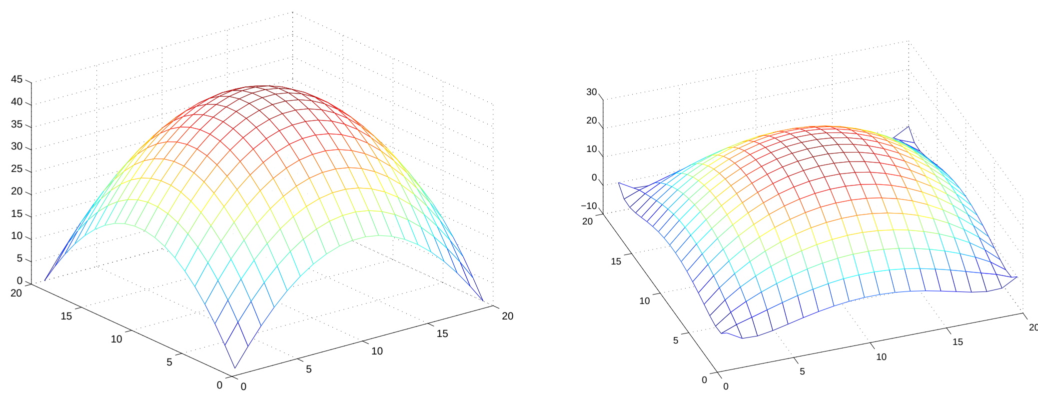
$\widetilde{W}_{\Pi}$ is " primal space" $=$ basis functions: one per crosspoint, edge, face
$\widetilde{W}_{\Delta} = \otimes \widetilde{W}_{\Delta i}, \quad \widetilde{W}_{\Delta i} = \{w_i \in W_i : C_i w_i = 0\}$ is the "dual space"

$$\begin{aligned}
\mathcal{F}(\lambda) &= \min_{u \in \widetilde{W}} \underbrace{\mathcal{E}(w) + w^T B^T \lambda}_{\mathcal{L}(u,\lambda)} \\
&= \min_{w_{\Pi} \in \widetilde{W}_{\Pi}} \left(\min_{w_{\Delta} \in \widetilde{W}_{\Delta}} \underbrace{\mathcal{E}(w_{\Pi} + w_{\Delta}) + (w_{\Pi} + w_{\Delta})^T B^T \lambda}_{\mathcal{L}(w_{\Pi}+w_{\Delta},\lambda)} \right)
\end{aligned}$$

Functions from primal and dual spaces

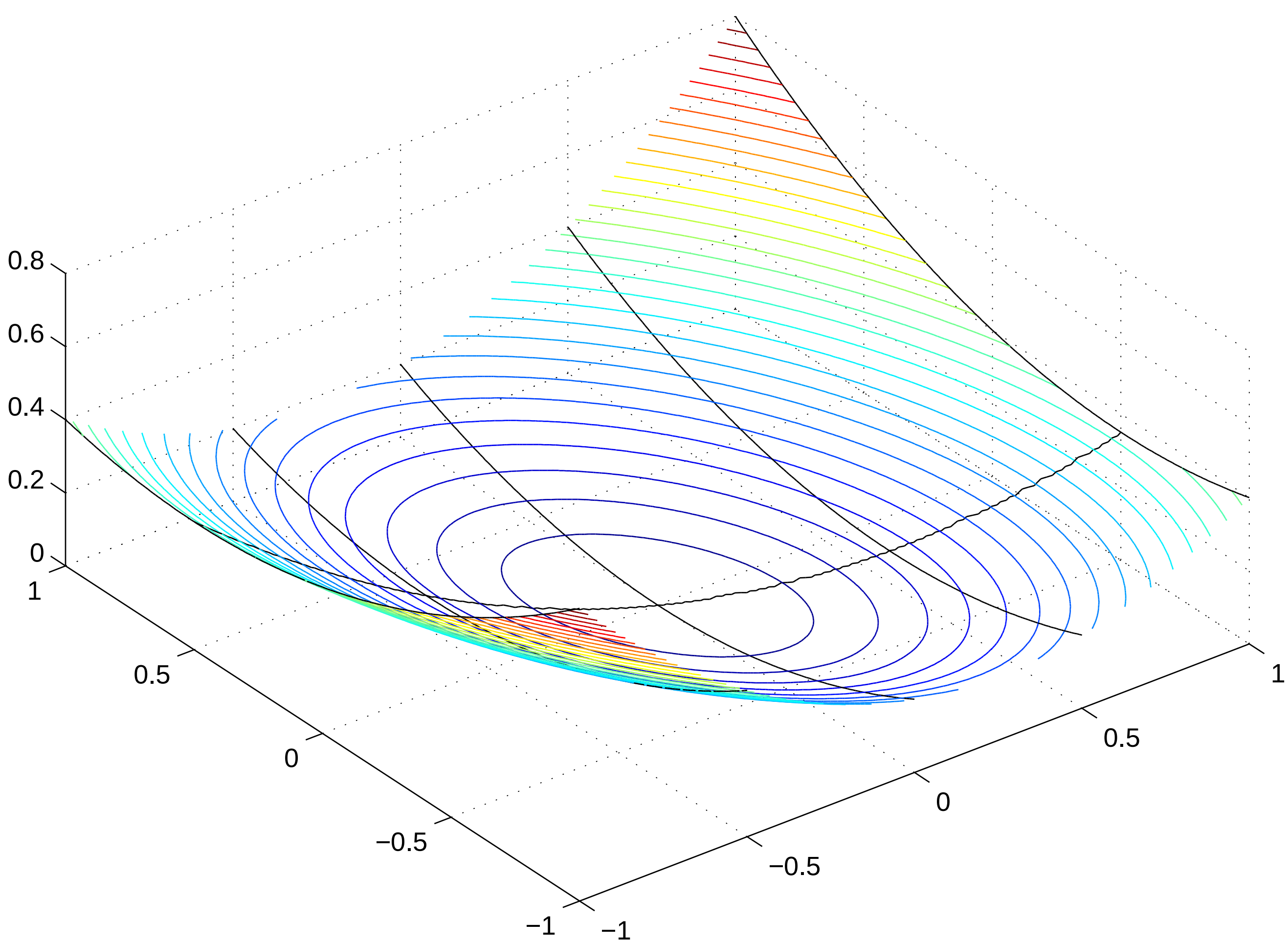


Basis functions of the primal (coarse) space $\widetilde{W}_{\Pi}$ (Klawonn, Widlund, Dryja 2002), 5-point Laplacian



Functions from $\widetilde{W}_{\Delta}$ with zero corner values, and zero corner values and edge averages

Nested minimization

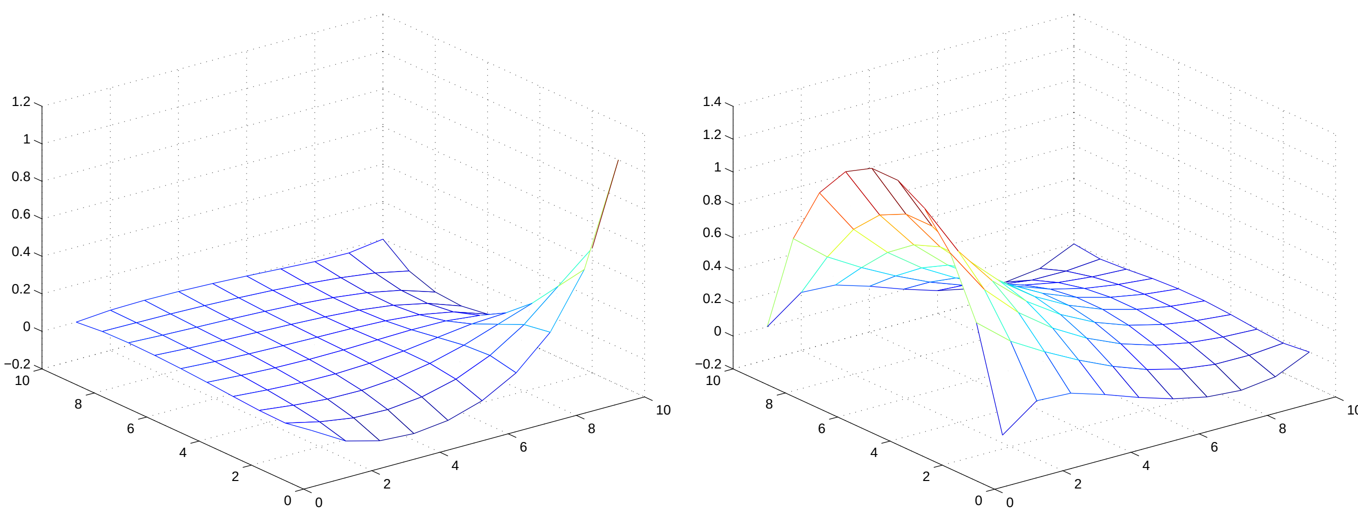


$$\widetilde{W} = \widetilde{W}_{\Pi} \oplus \widetilde{W}_{\Delta} \implies \min_{w \in \widetilde{W}} \mathcal{L}(w, \lambda) = \min_{w_{\Pi} \in \widetilde{W}_{\Pi}} \left(\min_{w_{\Delta} \in \widetilde{W}_{\Delta}} \mathcal{L}(w_{\Delta} + w_{\Pi}, \lambda) \right)$$

Coarse basis functions need not be continuous

In Klawonn, Windlund, Dryja 2002, the primal basis functions were assumed continuous, $B\widetilde{W}_{\Pi} = 0$ - needed for the condition number bounds. But $\mathcal{F}$ is defined by nested minimization $\implies$ we can take any $\widetilde{W}_{\Pi}$ such that $\widetilde{W} = \widetilde{W}_{\Pi} \oplus \widetilde{W}_{\Delta}$. More convenient $\widetilde{W}_{\Pi}$ for computations is by energy minimization, works for an arbitrary C:

$$\widetilde{W}_{\Pi} = \left\{ w \in W : C_i w_i = R_{ci} u_c,\ w_i^T K_i w_i \to \text{min} \right\}$$



A better FETI-DP Implementation

Dual problem: $\frac{\partial \mathcal{F}(\lambda)}{\partial \lambda} = 0$ where

$$\begin{aligned} \mathcal{F}(\lambda) &= \min_{w \in \widetilde{W}} \underbrace{\frac{1}{2} w^T S w - w^T g + w^T B^T \lambda}_{\mathcal{L}(w,\lambda)} \\ &= \min_{w_\Pi \in \widetilde{W}_\Pi} \left(\min_{w_\Delta \in \widetilde{W}_\Delta} \mathcal{L}(w_\Delta + w_\Pi, \lambda) \right) \end{aligned}$$

Eliminating $w_\Delta \implies$ solving N independent constrained problems

$$\begin{bmatrix} S_i & C_i^T \\ C_i & 0 \end{bmatrix} \begin{bmatrix} w_i \\ \varsigma_i \end{bmatrix} = \begin{bmatrix} f - B_i^T \lambda \\ 0 \end{bmatrix}$$

If there are enough corners $\implies$ constraints $(w_i)_j = 0 \implies$ SPD problem

These are the same constrained local problems as in BDDC.

Minimizing over $w_\Pi \in \widetilde{W}_\Pi \implies$ coarse problem is SPD, and also sparse

FETI-DP Algebraic Condition Bound

Theorem If $\forall w \in \widetilde{W} : \left\| B_D^T B w \right\|_S^2 \leq \omega \left\| u \right\|_S^2$,
then $\kappa_{\text{FETI-DP}} = \frac{\lambda_{\max}(MF)}{\lambda_{\min}(MF)} \leq \omega$.

Proof. The theory from Mandel and Tezaur 2001 goes through. ∎

Another useful form - subtract a continous interpolation u of w:

Corollary If $\forall w \in \widetilde{W} \exists u : Bu = 0, \left\| B_D^T B (w - u) \right\|_S^2 \leq \omega \left\| u \right\|_S^2$,
then $\frac{\lambda_{\max}(MF)}{\lambda_{\min}(MF)} \leq \omega$

This setting, and in particular use of the assumption $B B_D^T B = B$ was inspired by $\log^2 \frac{H}{h}$bounds from Klawonn, Widlund, Dryja 2002, which was in turn inspired by Mandel and Tezaur 2001. Brenner 2003: a setting and analysis of FETI-DP as an additive Schwarz method.

Evaluation of primal residual in FETI methods

The primal residual $r = R^T S R w - R^T g$ needed for stopping test
r can be evaluated along with the preconditioned residual
dual problem is $Bw = 0$, $w = w(\lambda) \implies$

residual of the dual problem	$g - \mathcal{F}\lambda = Bw$
preconditioned dual residual	$B_D S B_D^T (g - \mathcal{F}\lambda)$
residual of the primal problem	$r = R^T S B_D^T (g - \mathcal{F}\lambda)$

(algebraic generalization on mechanics based arguments from Rixen, Farhat 1999; relies on the identity $B_D^T B + R R^T D_P = I$)

BDDC: Balancing Domain Decomposition Based on Constraints

Reduction to Interfaces

Primal substructuring: iterate on the Schur complement system (standard since early 80s)

Substructure dof vectors on interfaces

$$w = \begin{bmatrix} w_1 \\ \vdots \\ w_N \end{bmatrix} \in W = W_1 \times \ldots \times W_N$$

substructure stiffness matrices reduced to interfaces S_i

local to global maps $R_i^T : W_i \to U$, $w_i = R_i u$, reduced RHS g_i

Problem to solve: $\sum_{i=1}^{N} R_i^T S_i R_i u = \sum_{i=1}^{N} R_i^T g_i$

Variational form: $u \in U : b(u,v) = v^T h \ \forall v \in V$

$$b(u,v) = \sum_{i=1}^{N} v^T R_i^T S_i R_i u$$

BDDC

Space decomposition and averaging on interfaces:

$U = U_0 \oplus U_1 \oplus \ldots \oplus U_N$

$U_i = \left\{ u_i = R_i^T D_i w_i : C_i w_i = 0 \right\}, \, i = 1, \ldots, N$

$U_0 = \left\{ u_0 = \sum_{i=1}^{N} (I - P) R_i^T D_i w_i : w_i^T K_i w_i \to \text{min s.t. } C_i w_i = R_{ci} u_c \right\}$

Bilinear forms: $b_i(u_i, u_i) = w_i^T K_i w_i, \qquad b_0(v_0, v_0) = \sum_{i=1}^{N} w_i^T K_i w_i$

Preconditioner is additive Schwarz:

$M : r \mapsto u = \sum_{i=0}^{N} u_i,$

$u_i \in U_i : b_i(v_i, u_i) = v_i^T r_i, \, \forall v_i \in U_i, \; i = 0, 1, \ldots, N.$

Note $U_0 = R^T D_P \widetilde{W}_\Pi, \, U_i = R_i^T D_{Pi} \widetilde{W}_{\Delta i}$

BDDC Algebraic Analysis

The BDDC method proposed by Dohrmann 2002. Schwarz formulation and analysis Mandel and Dohrmann 2002. Case of corner constraints only and $b_0 = b$ is identical to a Balancing Domain Decomposition variant by Le Tallec, Mandel, Vidrascu 1998

Abstract Additive Schwarz bounds (Dryja and Widlund 1995) and the identity $B_D^T B + RR^T D_P = I$ give here

Theorem. If If $\forall w \in \widetilde{W} : \left\| B_D^T B w \right\|_S^2 \leq \omega \|u\|_S^2$, then $\kappa_{\mathrm{BDDC}} \leq 5N_E(2 + 2\omega)$ where N_E is the maximum number of neighbors of any subdomain.

Conjecture. $\kappa_{\mathrm{BDDC}} = \kappa_{\mathrm{FETI-DP}} \leq \omega$

Standard substructuring arguments (Klawonn, Widlund, Dryja 2001) $\Longrightarrow$ $\omega \leq C \left(1 + \log^2 \frac{H}{h}\right)$

Computational setup

For comparison and analysis, both FETI-DP and BDDC implemented in Matlab

• controlled conditions for comparison, unlike production implementation in a big software package

• FETI-DP and BDDC implemented from identical components

• constraints: average of each field over each set of nodes that are adjacent to the same substructures

• weights: standard (Le Tallec, DeRoeck 1991) in proportion to diagonal stiffness:

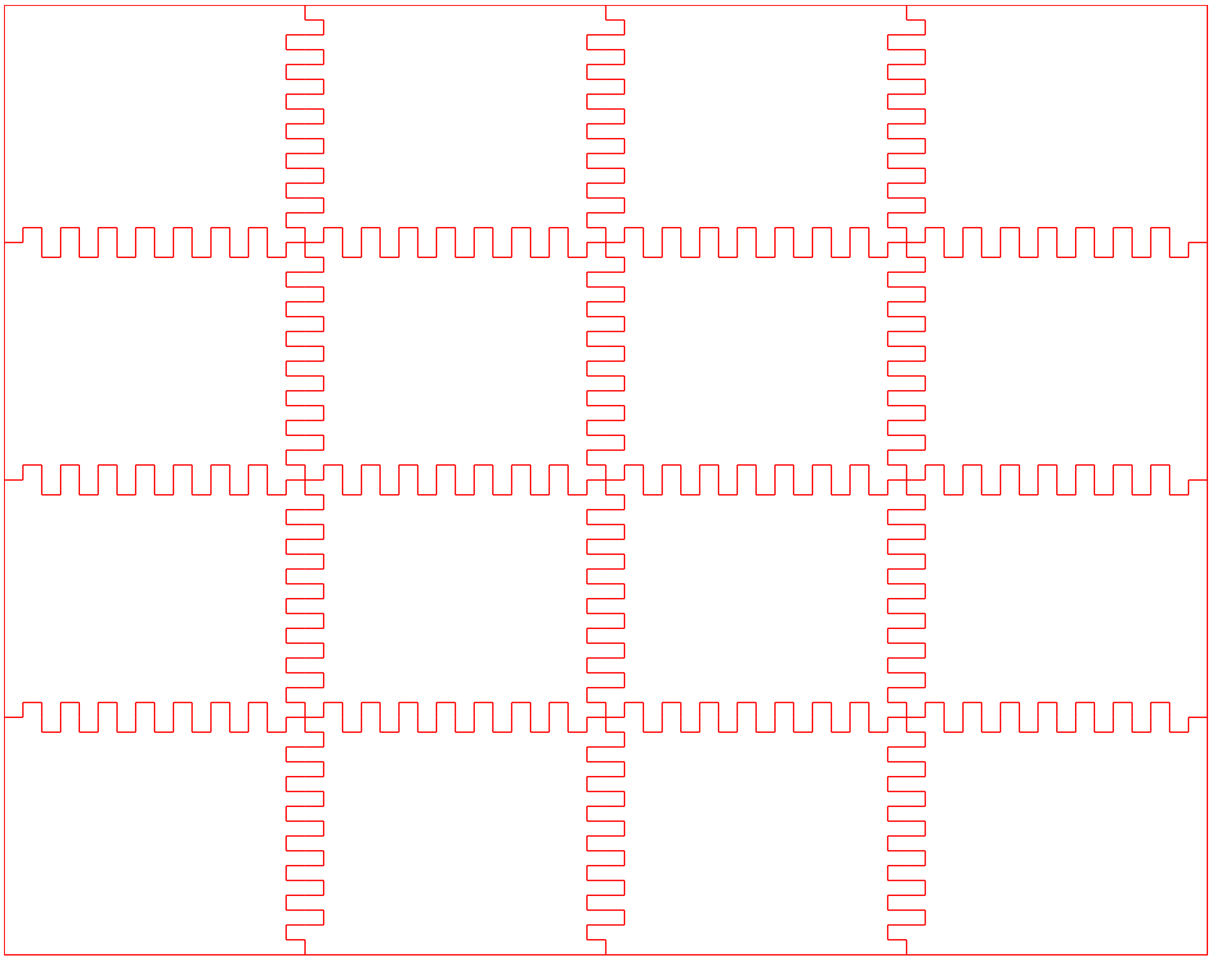
$$(D_{Pi})_{jj} = \frac{(K_i)_{jj}}{\sum\limits_{k:\Omega_k \text{ adjacent to } \Omega_i} (K_k)_{jj}}$$

• test problems: 2D and 3D elasticity on a regular mesh

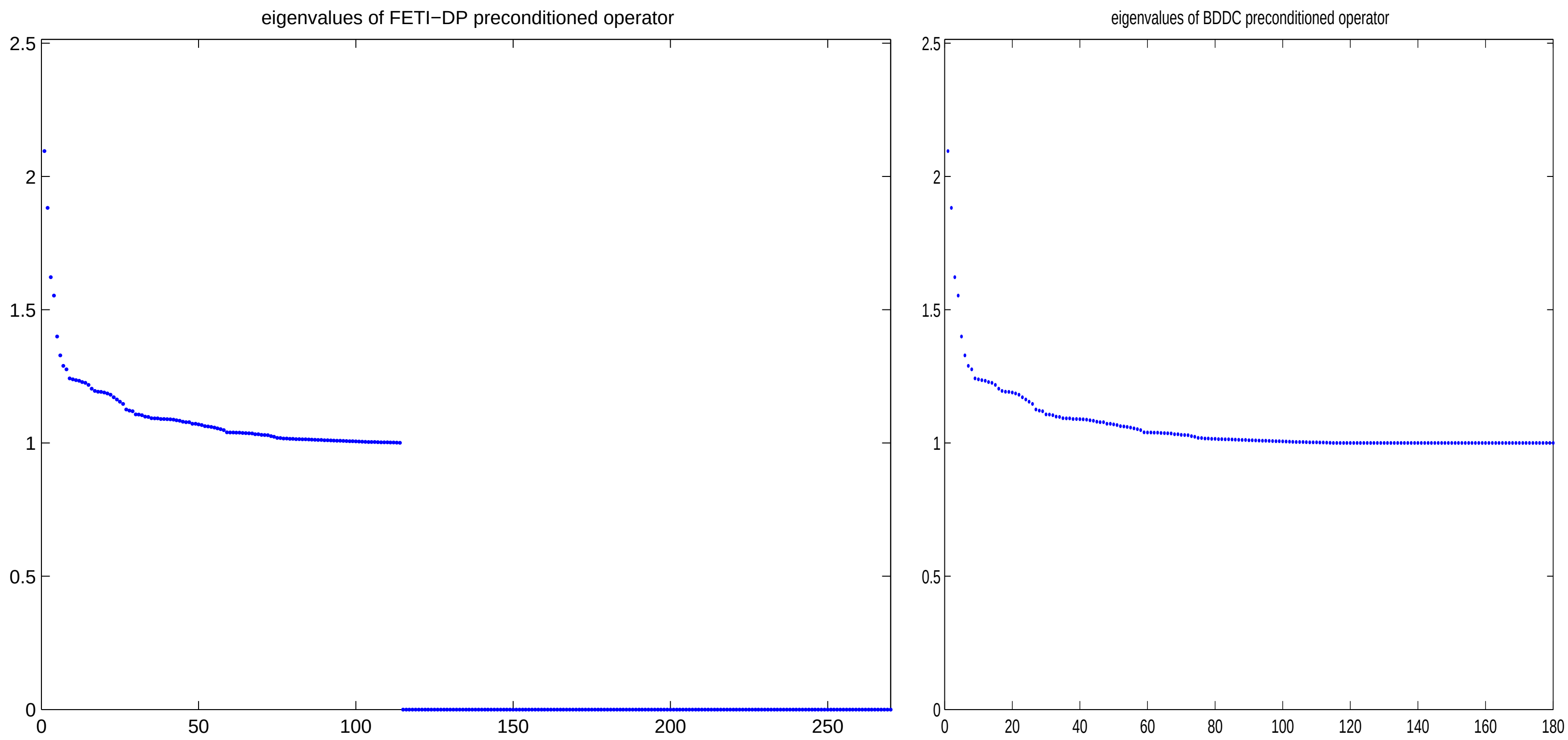
Computational results

			BDDC		FETI-DP	
name	ndof	nsub	niter	cond	niter	cond
square4x4Hh4	544	16	11	2.1	10	2.1
square4x4Hh8	2112	16	13	3.1	12	3.1
square4x4Hh16	8320	16	15	4.4	14	4.4
square4x4Hh32	33024	16	17	6.0	16	5.9
square4x4Hh64	131584	16	20	7.7	18	7.6
square4x4Hh4-jagged	544	16	27	9.3	27	9.1
square4x4Hh8-jagged	2112	16	44	22.0	45	21.6
square4x4Hh16-jagged	8320	16	49	33.8	50	33.2
square4x4Hh32-jagged	33024	16	54	58.0	52	57.0
square4x4Hh64-jagged	131584	16	61	107	59	105
square4x4-1e-4	1200	16	11	2.9	10	2.9
square4x4-1e-2	1200	16	11	2.9	10	2.9
square4x4-1e0	1200	16	10	2.7	9	2.6
square4x4-1e2	1200	16	10	2.2	9	2.2
square4x4-1e4	1200	16	11	2.2	10	2.2
cube4x4x4-1e-4	13872	64	14	2.8	13	2.8
cube4x4x4-1e-2	13872	64	14	2.8	13	2.8
cube4x4x4-1e0	13872	64	12	2.6	12	2.6
cube4x4x4-1e2	13872	64	12	2.3	11	2.3
cube4x4x4-1e4	13872	64	13	2.3	11	2.2

Square 4x4 H/h=16 jagged mesh



Eigenvalues of preconditioned operator



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

Brenner 2003: eigenvalues of FETI-DP ≥ 1 (the zeros are from redundant constraints in B)

Summary

- condition number bounds of FETI-DP reduced to a single inequality in terms of problem matrices
  $\Longrightarrow$ foundation of adaptive methods

- existing FEM theory $\Longrightarrow$ $\log^2 \frac{H}{h}$ asymptotic bounds

- alternative formulation of FETI-DP with general constraints and requiring solution of SPD systems only

- with identical components (constraints, weights) FETI-DP and BDDC performs very similarly, and the sets of eigenvalues of the respective preconditioned operators are identical

Future directions

- bounds in the case of weights not constrant along edges
- prove the conjecture that the spectra of FETI-DP and BDDC equal
- coarse problem solved by the same method, multilevel estimates (as a multilevel Schwarz method)
- choose constraints to make the estimates small $\Longrightarrow$ robust adaptive methods
- elasticity, minimize the number of needed constraints (Klawonn, Dryja, Widlund) then use the saved work where it is needed to improve convergence