

Multilevel and Adaptive Iterative Substructuring Methods

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The multilevel BDDC method is joint work with Bedřich Sousedík, Czech Technical University, and Clark Dohrmann, Sandia. The adaptive BDDC method is joint work with Bedřich Sousedík. BDDC implementation on top of frontal solver is joint work with Jakub Šístek, Jaroslav Novotný, Marta Čertíková, and Pavel Burda, Czech Technical University.

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A Somewhat Biased Short Overview of Iterative Substructuring a.k.a. Nonoverlapping DD

- assemble elements into substructures, eliminate interiors \implies reduced problem (Schur complement) on interface (Dirichlet-to-Neumann operator $H^{1/2} \rightarrow H^{-1/2}$, a.k.a. Poincaré-Steklov operator)

$$\text{cond} \approx O\left(\frac{\text{number of substructures}^2 * \text{substructure size}}{\text{mesh step (=element size)}}\right) = O(N^2) O\left(\frac{H}{h}\right)$$

- for parallel solution; Schur complement matrix-vector multiply = solve substructure Dirichlet problem
- only matrix datastructures needed; condition number $O(1/h)$ better in practice than the $O(1/h^2)$ for the original problem (for small N)

Early Preconditioners

- diagonal preconditioning: Gropp and Keyes 1987, “probing” the diagonal of the Schur complement Chan and Mathew 1992 (because creating the diagonal of the Schur complement is expensive)...
- preconditioning by solving substructure Neumann problems ($H^{-1/2} \rightarrow H^{1/2}$) Glowinski and Wheeler 1988, Le Talleck and De Roeck 1991 (a.k.a. the Neumann-Neumann method)
- optimal substructuring methods: coarse problem: $O(N^2) \rightarrow \text{const}$, asymptotically optimal preconditioners $H/h \rightarrow \log^2(1 + H/h)$ (Bramble, Pasciak, Schatz 1986+, Widlund 1987, Dryja 1988,... **but all these methods require access to mesh details and depend on details of the Finite Element code, which makes them hard to implement in a professional software framework**)

FETI and BDD

- algebraic - need only substructure 1. solvers (Neumann, Dirichlet), 2. connectivity, 3. basis of nullspace (BDD - constant function for the Laplacian, FETI - actual nullspace)
- both involve singular substructure problems (Neumann) and build the coarse problem from local substructure nullspaces (in different ways) to assure that the singular systems are consistent
- Balancing Domain Decomposition (BDD, Mandel 1993): solve the system reduced to interfaces, interface degrees of freedom common (this is the Neumann-Neumann with a particular coarse space)
- Finite Element Tearing and Interconnecting (FETI, Farhat and Roux 1991): enforce continuity across interfaces by Lagrange multipliers, solve the dual system for the multipliers

FETI and BDD Developments

- Both methods require only matrix level information that is readily available in Finite Element software (no fussing with the meshes, coordinates, and individual elements...) and can be implemented easily outside of the FE engine. So they became very popular and widely used. The methods work well in 2D and 3D (solids).
- But the performance for plates/shells/biharmonic not so good. Reason: the condition numbers depend on the energy (trace norm) of functions with jumps across a substructure corner. In 2D, OK for $H^{1/2}$ traces of H^1 functions, not $H^{3/2}$ traces of H^2 functions (embedding theorem).
- Fix: avoid this by increasing the coarse space and so restricting the space where the method runs, to **make sure that nothing gets torn across the corners** (BDD: LeTallec Mandel Vidrascu 1998, FETI: Farhat Mandel 1998, Farhat Mandel Tezaur 1998). Drawback: complicated, expensive, a large coarse problem with custom basis functions

State of the Art: FETI-DP and BDDC

- To assure that nothing gets torn across the corners, enforce identical values at corners from all neighboring substructures a-priori \implies corner values are coarse degrees of freedom
- Continuity elsewhere at the interfaces by Lagrange multipliers as in FETI \implies FETI-DP (Farhat et al 2001)
- Continuity elsewhere by common values as in BDD \implies BDDC (Dohrmann 2003; independently Cros 2003, Frakagis and Papadrakakis 2003, with corner coarse degrees of freedom only)
- **Additional coarse degrees of freedom (side/face averages)** required in 3D for good conditioning: Farhat, Lesoinne, Pierson 2000 (algorithm only), Dryja Windlud 2002 (with proofs)

BDDC = Balancing Domain Decomposition by Constraints

- Coarse space from energy optimal functions, discontinuous between substructures, given by coarse dofs.
- Local spaces defined by coarse dofs equal to zero.
- In the case of corner coarse dofs only, these are the same spaces as in one variant of BDD for plates by LeTallec, Mandel, Vidrascu (1995, 1998).
- But in BDDC, the coarse correction is done additively not multiplicatively \implies great simplification, reduced complexity (number of nonzeros in the coarse matrix)
- The BDDC framework also allows more general coarse dofs than values at corners, namely the averages.

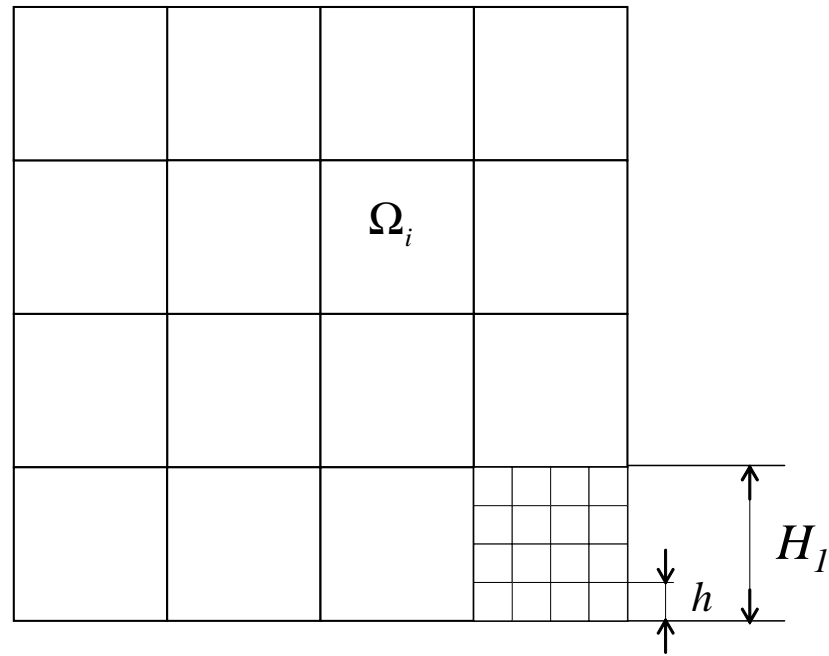
Connections between FETI and BDD, and FETI-DP and BDDC

- BDD and FETI are conceptually dual but it was long time unclear how exactly.
- First algebraic connection between BDD averaging and FETI jump operators (Rixen, Farhat, Tezaur, Mandel 1999)
- Common condition number bound by the energy norm of the averaging operator for FETI and BDD (Klawonn and Widlund 2001)
- Collected the algebraic relations, formulated primal versions of FETI, FETI-DP (Fragakis Papadralakis 2003)

Connections between FETI and BDD, and FETI-DP and BDDC (cont.)

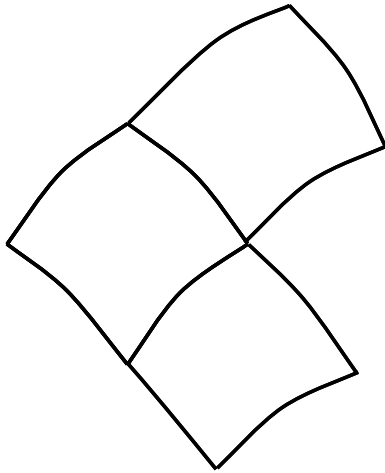
- Same condition number bound by energy norm of the averaging operator for FETI-DP (Mandel and Tezaur 2001) and BDDC (Mandel and Dohrmann 2003)
- **The eigenvalues of the preconditioned FETI-DP and BDDC operators are the same** (Mandel, Dohrman, and Tezaur 2005, simplified proofs: Li and Widlund 2006, Brenner and Sung 2007, Mandel and Sousedik 2007)
- Complete algebraic theory linking FETI and BDD, FETI-DP and BDDC, and their condition number bounds (Fragakis 2007, Sousedik and Mandel 2008)

Substructuring for a Problem with $H/h=4$



BDDC Description - Example Spaces

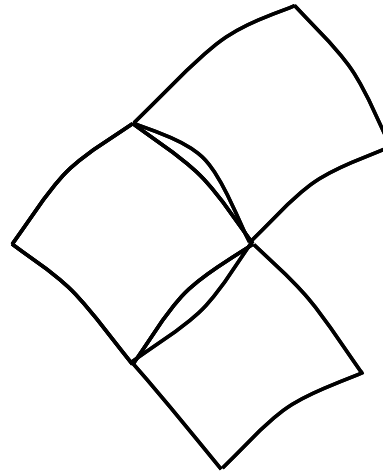
$W = \bigotimes_{i=1}^N W_i$: space of block vectors, one block per substructure



U

continuous across whole
substructure interfaces
global matrix: assembled
substructures: assembled

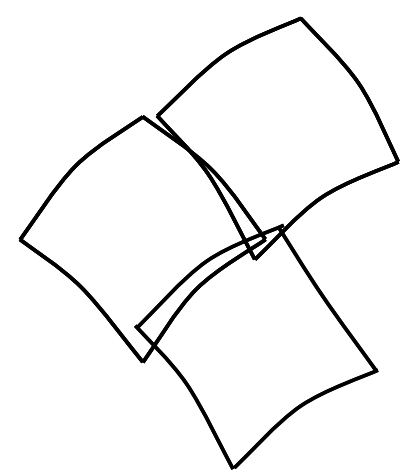
\subset



\tilde{W}

continuous across
corners only
partially assembled
assembled

\subset



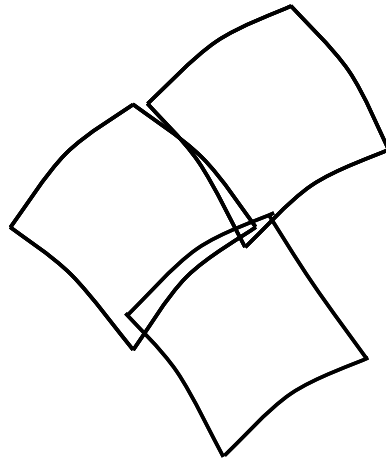
W

no continuity
required
not assembled
assembled

Want to solve: $u \in U : a(u, v) = \langle f, v \rangle \quad \forall v \in U, a(\cdot, \cdot)$ SPD on U
 $a(\cdot, \cdot)$ defined on the bigger space W

BDDC Description - Example Form and RHS

$W = \bigotimes_{i=1}^N W_i$: space of block vectors, one block per substructure Ω_i ,
 $w = (w_i)$



The bilinear form a and the right-hand side f defined by integrals over substructures:

$$a(w, v) = \sum_{i=1}^N \int_{\Omega_i} \nabla w_i \nabla v_i, \quad \langle f, v \rangle = \sum_{i=1}^N \int_{\Omega_i} f_i v_i$$

Abstract BDDC (Two Levels): Variational Setting of the Problem and Algorithm Components

$$u \in U : a(u, v) = \langle f, v \rangle, \quad \forall v \in U$$

$a(\cdot, \cdot)$ SPD on U and **positive semidefinite** on $W \supset U$, $\langle \cdot, \cdot \rangle$ is inner product

Example:

$W = W_1 \times \cdots \times W_N$ (spaces on substructures)

$U =$ functions continuous across interfaces

Choose preconditioner components:

space \widetilde{W} , $U \subset \widetilde{W} \subset W$, such that a is positive definite on \widetilde{W} .

Example: functions with continuous coarse dofs, such as values at substructure corners

projection $E : \widetilde{W} \rightarrow U$, $\text{range } E = U$.

Example: averaging across substructure interfaces

Abstract BDDC Preconditioner

Given a on $W \supset U$, define $A : U \rightarrow U$ by $a(v, w) = \langle Av, w \rangle \quad \forall v, w \in U$
Choose \widetilde{W} such that $U \subset \widetilde{W} \subset W$, and projection $E : \widetilde{W} \rightarrow U$ onto

Theorem 1 **The abstract BDDC preconditioner** $M : U \rightarrow U$,

$$M : r \longmapsto u = Ew, \quad w \in \widetilde{W} : \quad a(w, z) = \langle r, Ez \rangle, \quad \forall z \in \widetilde{W},$$

satisfies

$$\kappa = \frac{\lambda_{\max}(MA)}{\lambda_{\min}(MA)} \leq \omega = \sup_{w \in \widetilde{W}} \frac{\|Ew\|_a^2}{\|w\|_a^2}.$$

In implementation, \widetilde{W} is decomposed (energy orthogonal!)

$$\widetilde{W} = \widetilde{W}_{\Delta} \oplus \widetilde{W}_{\square}$$

\widetilde{W}_{Δ} = functions with zero coarse dofs \Rightarrow local problems on substructures

\widetilde{W}_{\square} = coarse space, functions given by coarse dofs & energy minimal

\Rightarrow global coarse problem

BDDC Implementation on Top of Frontal Solver

(Šístek, Novotný, Mandel, Čertíková, Burda, 2008)

Frontal solver: Solve linear equations from finite elements with some variables free and some constrained. Matrix given as a collection of local element matrices, never assembled whole.

In: f_1 x_2 Out: x_1 Rea

$$\begin{bmatrix} A_{11} & A_{12} \\ A_{21} & A_{22} \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \end{bmatrix} = \begin{bmatrix} f_1 \\ 0 \end{bmatrix} + \begin{bmatrix} 0 \\ Rea \end{bmatrix}$$

Straightforward to use the frontal solver to:

- solve the coarse problem in BDDC (substructure treated as element)
- solve the local substructure problems in BDDC in the case of corner constraints only

New: by specially crafted calls and few extras, use the frontal solver to

- solve the local substructure problems in BDDC in the case of general constraints (averages)
- build the coarse basis functions

Adaptive BDDC

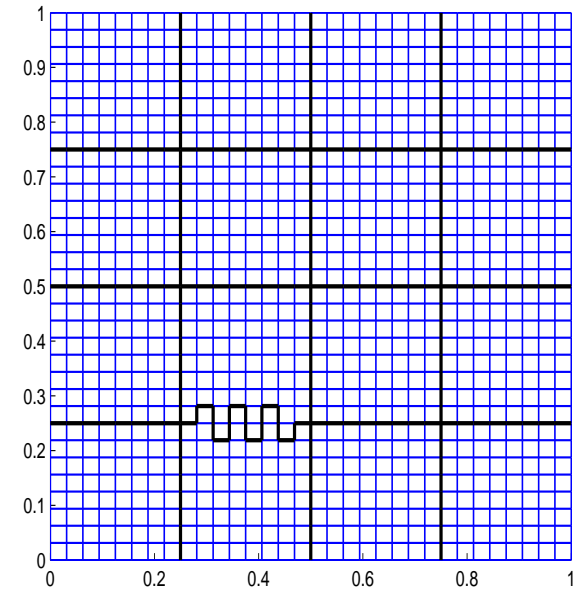
(Mandel, Sousedík, 2007)

- Enrich coarse space: add averages on edges (2D), sides (3D)
- Condition number is a Rayleigh quotient on subspace \widetilde{W} : optimal enrichment should cause \widetilde{W} to be orthogonal to the dominant eigenvectors
- But the eigenvectors and the added coarse basis functions are global: expensive
- Use eigenvectors of adjacent pairs of substructures: practical heuristic method
- Adds a variable number of constraints by weighted averages

Adaptive Coarse DOFs for Plane Elasticity

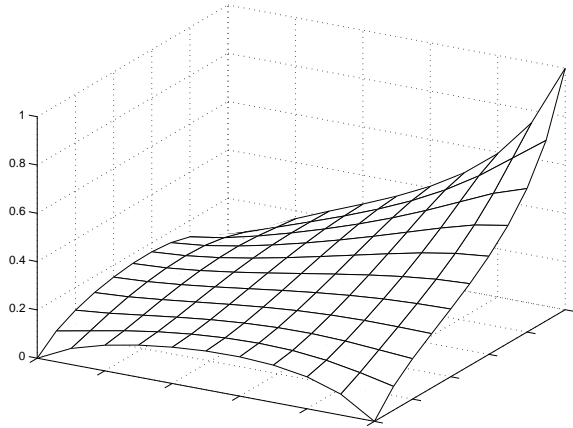
$$\lambda = 1 \quad \mu = 2$$

H/h	Ndof	τ	Nc	$\tilde{\omega}$	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
8	2178		42	17	17	28
		10	45	9.4	9.4	25
		3	59	2.9	4.0	20
		2	82	2.0	2.6	15
16	8450		42	22	20	37
		10	50	8.7	9.9	29
		3	77	<3	4.6	22
		2	112	<2	2.6	15
32	33282		42	41	20	45
		10	60	<10	9.5	33
		3	108	<3	4.7	21
		2	134	<2	2.9	17
64	132098		42	87	40	55
		10	89	<10	9.9	36
		3	151	<3	4.7	22
		2	174	<2	2.9	17



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

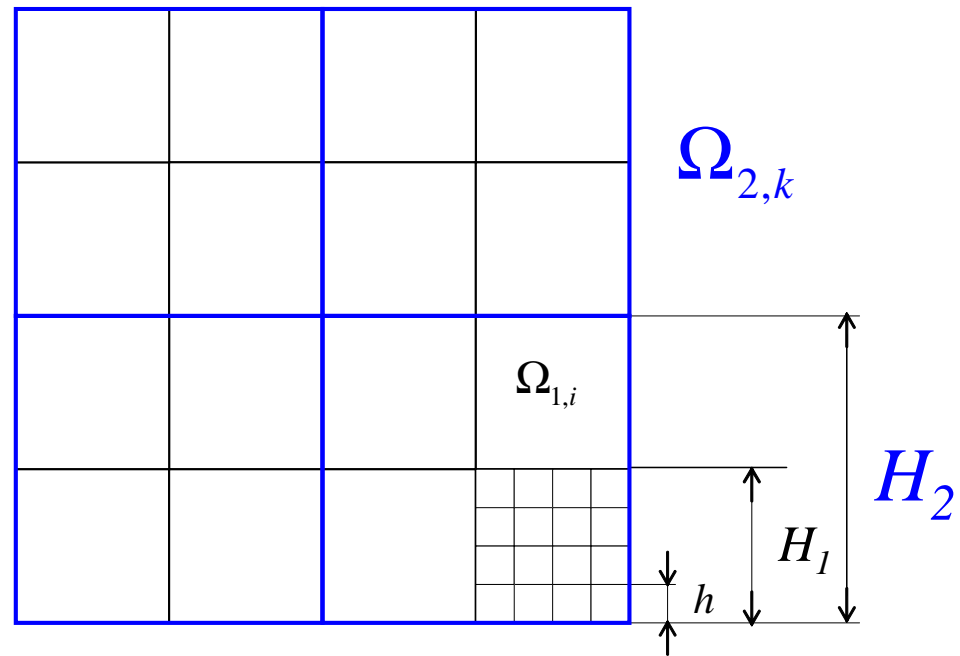
The Coarse Problem



A basis function from \widetilde{W}_Π is energy minimal subject to given values of coarse degrees of freedom on the substructure. The function is discontinuous across the interfaces between the substructures but the values of coarse degrees of freedom on the different substructures coincide.

- **For large problems, the coarse problem is a bottleneck.**
- The coarse problem has the same structure as the original FE problem \implies solve it approximately by one iteration of BDDC \implies three-level BDDC (Tu 2004, 2005)
- Apply recursively \implies **multi-level BDDC**

Substructuring for a Three-level Model Problem



Abstract Multispace BDDC

Choose a space with **decomposition** $\sum_{k=1}^N V_k$ and **projections** Q_k as

$$U \subset \sum_{k=1}^N V_k \subset W, \quad Q_k : V_k \rightarrow U$$

V_k energy orthogonal: $V_k \perp_a V_\ell, k \neq \ell,$

$$\text{assume } \forall u \in U : \left[u = \sum_{k=1}^N v_k, v_k \in V_k \right] \implies u = \sum_{k=1}^N Q_k v_k$$

Equivalently, assume $\Pi_k : \bigoplus_{j=1}^M V_j \rightarrow V_k$ are a -orthogonal projections, and

$$I = \sum_{k=1}^N Q_k \Pi_k \text{ on } U$$

Abstract Multispace BDDC

Theorem 2 **The abstract Multispace BDDC preconditioner** $M : U \longrightarrow U$ defined by

$$M : r \mapsto u, \quad u = \sum_{k=1}^N Q_k v_k, \quad v_k \in V_k : \quad a(v_k, z_k) = \langle r, Q_k z_k \rangle, \quad \forall z_k \in V_k,$$

satisfies

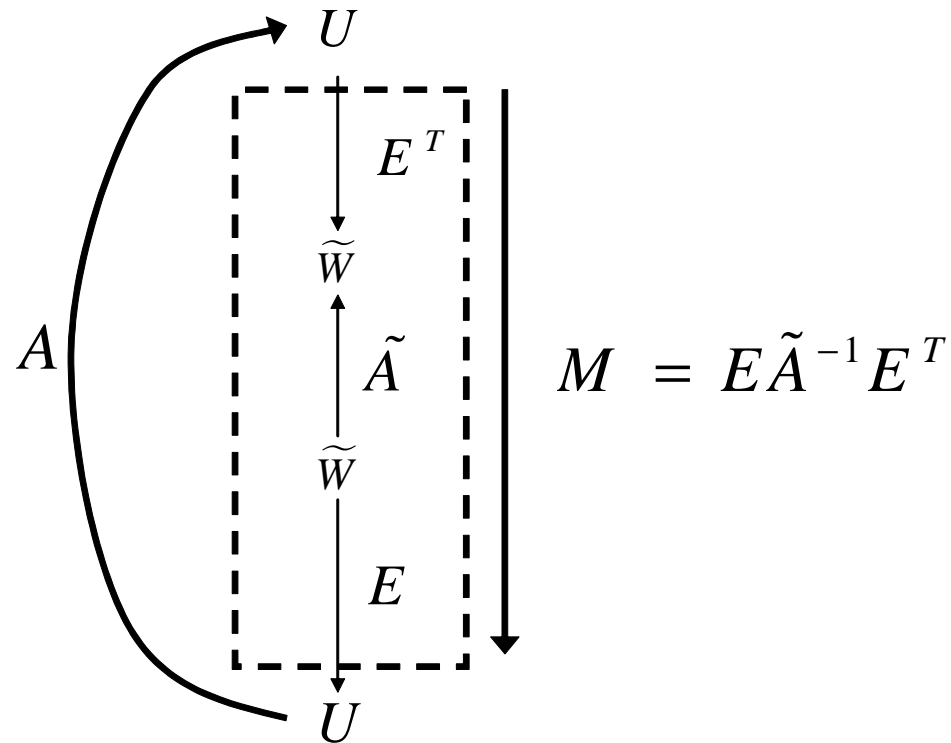
$$\kappa = \frac{\lambda_{\max}(MA)}{\lambda_{\min}(MA)} \leq \omega = \max_k \sup_{v_k \in V_k} \frac{\|Q_k v_k\|_a^2}{\|v_k\|_a^2}.$$

For $N = 1$ we recover the abstract BDDC algorithm and condition number bound. Proved from generalized Schwarz theory (Dryja and Widlund, 1995). Unlike in the Schwarz theory, we decompose some space larger than U .

In a sense:

1. the spaces V_k decompose the space \widetilde{W} , and
2. the projections $Q_k : V_k \rightarrow U$ decompose the projection $E : \widetilde{W} \rightarrow U$.

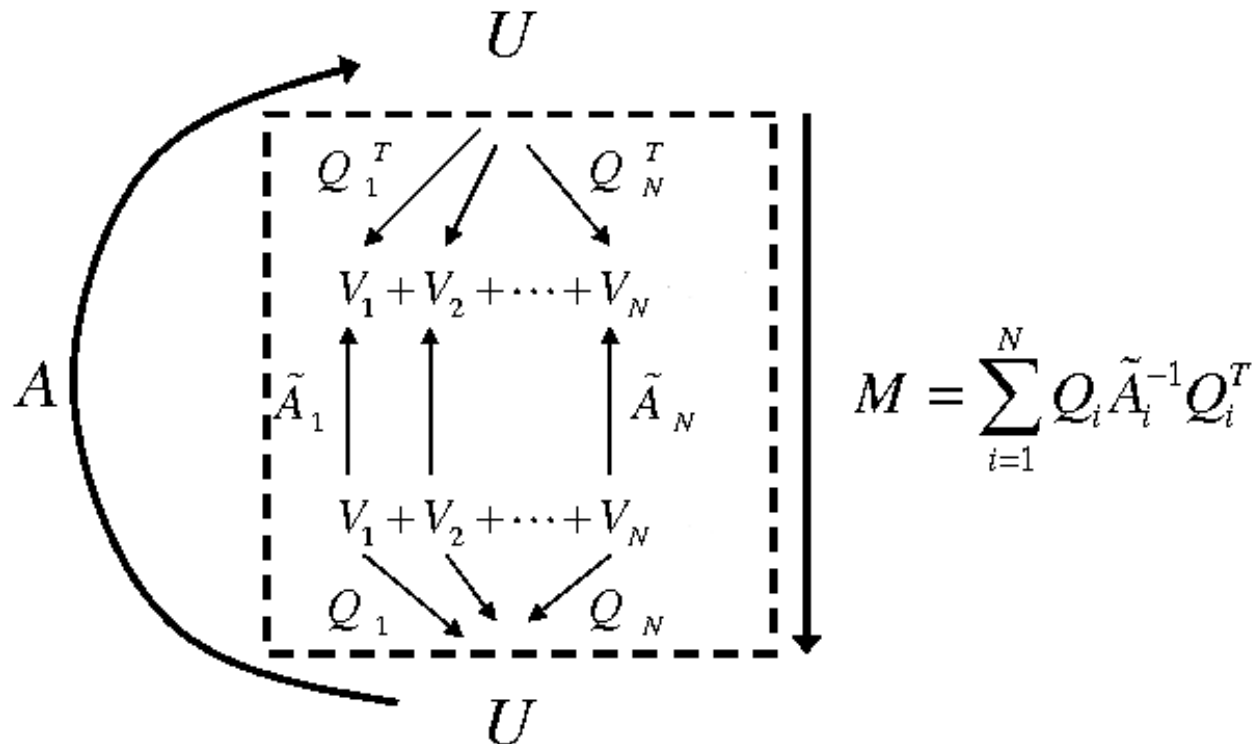
Algebraic View of the Abstract BDDC Preconditioner



The same bilinear form a defines $A : U \rightarrow U$ and $\tilde{A} : \tilde{W} \rightarrow \tilde{W} \supset U$

The preconditioner M to A is obtained by solving a problem with the same bilinear form on the bigger space \tilde{W} and mapping back to U via the projection E and its transpose E^T .

Algebraic View of the Abstract Multispace BDDC Preconditioner



The same bilinear form a defines $A : U \rightarrow U$ and $\tilde{A}_i : V_i \rightarrow V_i$, $\sum_{i=1}^N V_i \supset U$

The preconditioner M to A is obtained by solving problems with the same bilinear form on the bigger spaces V_i and mapping back to U via the projections Q_i and their transposes Q_i^T .

BDDC with Interiors as Multispace BDDC

Abstract BDDC often presented on the space of discrete harmonic functions. The original BDDC formulation had “interior correction”:

$$\boxed{U_I \begin{array}{c} P \\ \leftarrow \\ \subset \end{array} U \begin{array}{c} E \\ \leftarrow \\ \subset \end{array} \widetilde{W}}$$

Lemma 3 *The original BDDC preconditioner is the abstract Multispace BDDC method with $N = 2$ and the spaces and operators*

$$V_1 = U_I, \quad V_2 = (I - P)\widetilde{W}, \quad Q_1 = I, \quad Q_2 = (I - P)E.$$

The space \widetilde{W} has an α -orthogonal decomposition

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

so the problem on \widetilde{W} splits into independent problems on \widetilde{W}_Δ and \widetilde{W}_Π .

Example:

\widetilde{W}_Δ = functions zero on substructure corners

\widetilde{W}_Π = given by values on substructure corners and energy minimal

BDDC with Interiors as Multispace BDDC

The same BDDC formulation with “interior correction” and splitting of \widetilde{W} :

$$\begin{array}{c}
 U_I \xleftarrow{P} U \xleftarrow{E} \widetilde{W} \\
 \xleftarrow{C} \qquad \qquad \qquad \parallel \\
 \qquad \qquad \qquad \widetilde{W}_\Pi \oplus \widetilde{W}_\Delta
 \end{array}$$

Lemma 4 *The original BDDC preconditioner is the abstract multi-space BDDC method with $N = 3$ and the spaces and operators*

$$V_1 = U_I, \quad V_2 = \widetilde{W}_\Pi, \quad V_3 = (I - P)\widetilde{W}_\Delta, \quad Q_1 = I, \quad Q_2 = Q_3 = (I - P)E.$$

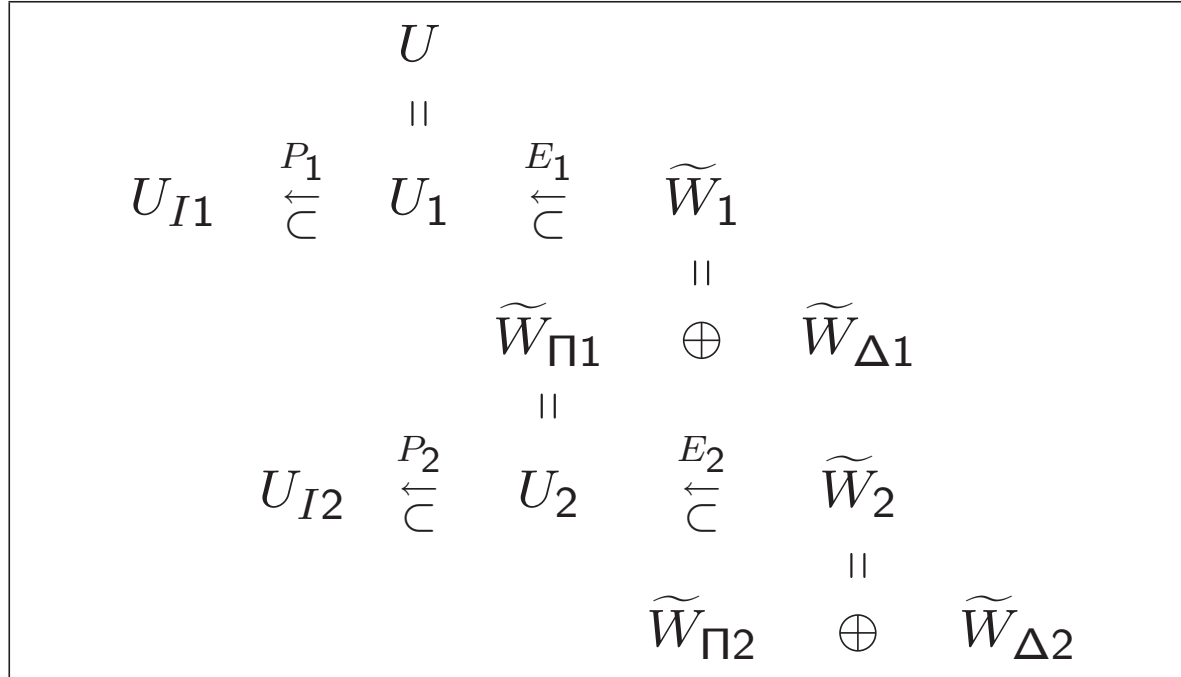
Solving on $U_I \Rightarrow$ independent Dirichet problems on substructures

Solving on $(I - P)\widetilde{W}_\Delta \Rightarrow$ independent constrained Neumann problems on substructures + correction in U_I

Solving on $\widetilde{W}_\Pi \Rightarrow$ **Global coarse problem with substructures as coarse elements and energy minimal function as coarse shape functions.**

Three-level BDDC

Coarse problem solved approximately by the BDDC preconditioner.

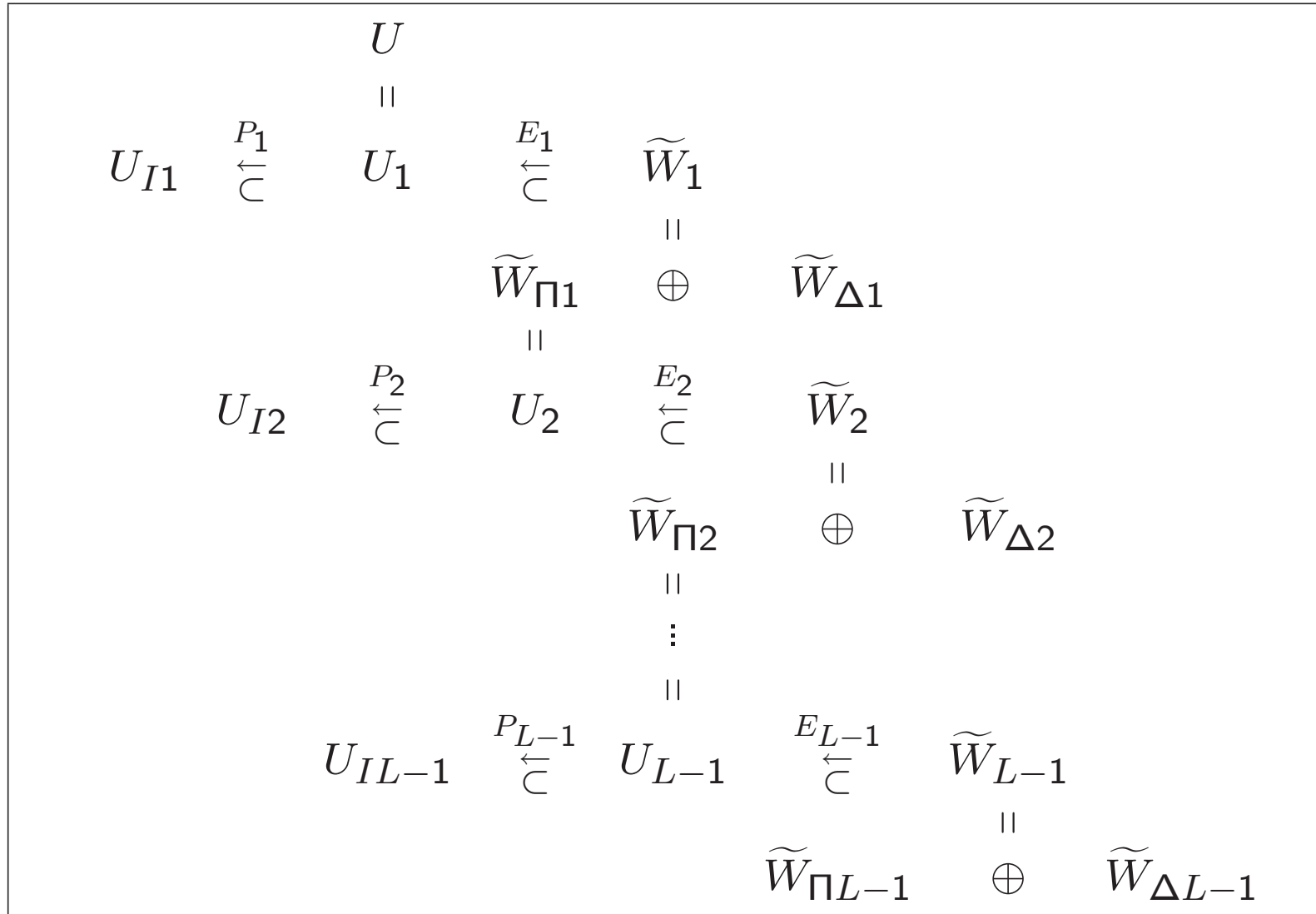


Lemma 5 *The three-level BDDC preconditioner is the abstract Multispace BDDC method with $N = 5$ and the spaces and operators*

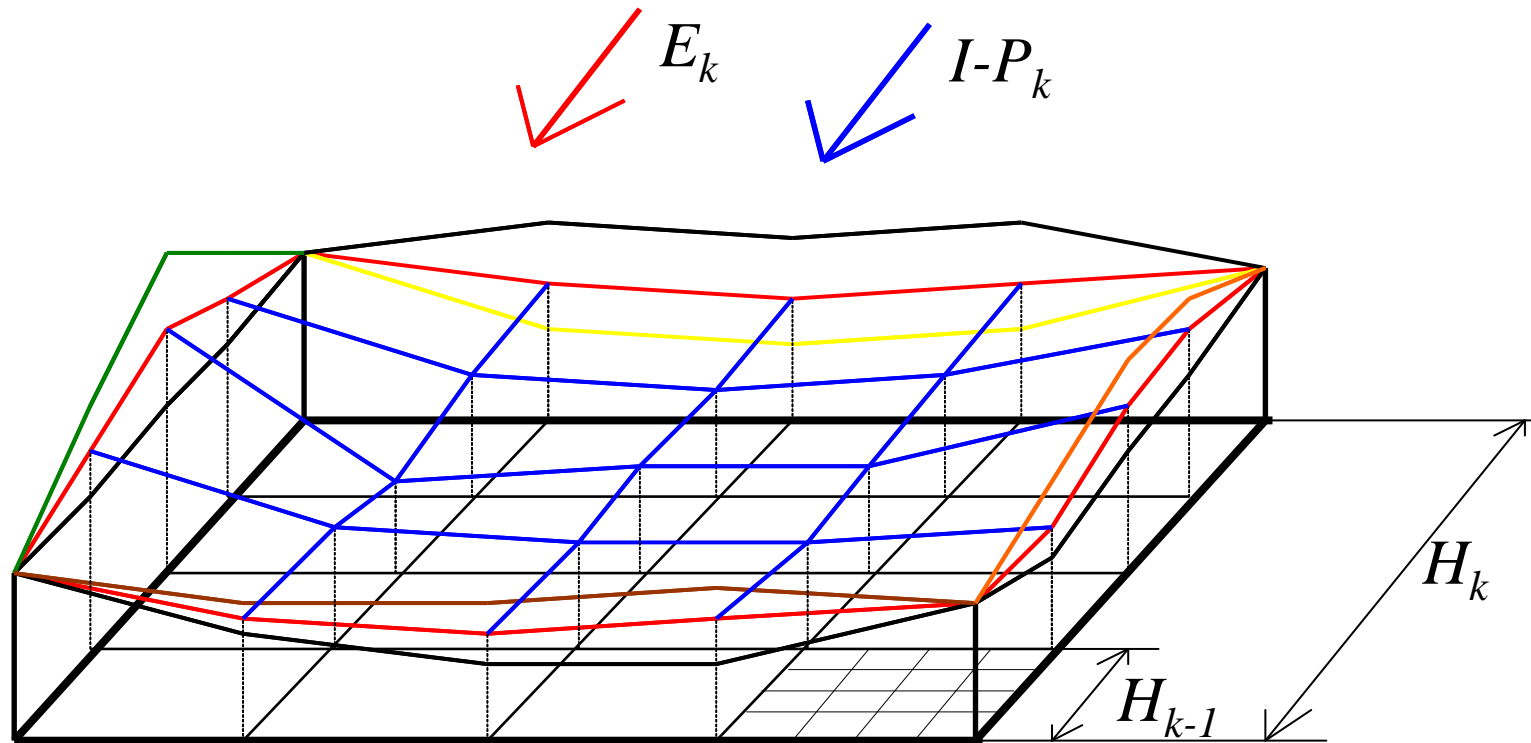
$$\begin{aligned}
 V_1 &= U_{I1}, & V_2 &= (I - P_1)\widetilde{W}_{\Delta 1}, & V_3 &= U_{I2}, & V_4 &= (I - P_2)\widetilde{W}_{\Delta 2}, & V_5 &= \widetilde{W}_{\Pi 2}, \\
 Q_1 &= I, & Q_2 &= Q_3 = (I - P_1)E_1, & Q_4 &= Q_5 = (I - P_1)E_1(I - P_2)E_2.
 \end{aligned}$$

Multilevel BDDC

Coarse problem solved by the BDDC preconditioner, recursive.



An Example of the Action of Operators E_k and $I - P_k$



Values on this substructure and its neighbors are **averaged by E_k** , then **extended as “discrete harmonic” by $I - P_k$** .

Basis functions on level k are given by dofs on level k & **energy minimal** w.r.t. basis functions on level $k - 1$. **Discrete harmonics** on level k are given by boundary values & **energy minimal** w.r.t. basis functions on level $k - 1$.

Multilevel BDDC

Coarse problem solved by the BDDC preconditioner, recursive.

Lemma 6 *The Multilevel BDDC preconditioner is the abstract Multispace BDDC preconditioner with $N=2L-2$ and*

$$\begin{aligned}
 V_1 &= U_{I1}, & V_2 &= (I - P_1)\widetilde{W}_{\Delta 1}, & V_3 &= U_{I2}, \\
 V_4 &= (I - P_2)\widetilde{W}_{\Delta 2}, & V_5 &= U_{I3}, & \dots \\
 V_{2L-4} &= (I - P_{L-2})\widetilde{W}_{\Delta L-2}, & V_{2L-3} &= U_{IL-1}, \\
 V_{2L-2} &= (I - P_{L-1})\widetilde{W}_{L-1} \\
 Q_1 &= I, & Q_2 &= Q_3 = (I - P_1) E_1, \\
 Q_4 &= Q_5 = (I - P_1) E_1 (I - P_2) E_2, & \dots \\
 Q_{2L-4} &= Q_{2L-3} = (I - P_1) E_1 \cdots (I - P_{L-2}) E_{L-2}. \\
 Q_{2L-2} &= (I - P_1) E_1 \cdots (I - P_{L-1}) E_{L-1}
 \end{aligned}$$

Recall condition number bound:

$$\kappa = \frac{\lambda_{\max}(MA)}{\lambda_{\min}(MA)} \leq \omega = \max_k \sup_{v_k \in V_k} \frac{\|Q_k v_k\|_a^2}{\|v_k\|_a^2}.$$

Algebraic Condition Estimate of Multilevel BDDC

Lemma 7 *If*

$$\|(I - P_1)E_1w_1\|_a^2 \leq \omega_1 \|w_1\|_a^2 \quad \forall w_1 \in \widetilde{W}_1,$$

$$\|(I - P_2)E_2w_2\|_a^2 \leq \omega_2 \|w_2\|_a^2 \quad \forall w_2 \in \widetilde{W}_2,$$

\vdots

$$\|(I - P_{L-1})E_{L-1}w_{L-1}\|_a^2 \leq \omega_{L-1} \|w_{L-1}\|_a^2 \quad \forall w_{L-1} \in \widetilde{W}_{L-1}.$$

then the multilevel BDDC preconditioner satisfies $\kappa \leq \prod_{i=1}^{L-1} \omega_i$.

- All spaces are subspaces of the single space W .
- The functions $(I - P_i)E_iw_i$ are discrete harmonic functions on level i with energy minimal extension into the interior after averaging on level i , such that w_i has continuous coarse dofs (such as values at corners) at the decomposition level $i - 1$.

Condition Number Estimate with Corner Constraints

Theorem 8 *The Multilevel BDDC preconditioner in 2D with corner constraints only satisfies*

$$\kappa \leq C_1 \left(1 + \log \frac{H_1}{h}\right)^2 C_2 \left(1 + \log \frac{H_2}{H_1}\right)^2 \cdots C_{L-1} \left(1 + \log \frac{H_{L-1}}{H_{L-2}}\right)^2 .$$

For $L = 3$ we recover the estimate by Tu (2004).

This bound implies at most polylogarithmic growth of the condition number in the ratios of mesh sizes for a fixed number of levels L

For fixed H_i/H_{i-1} the growth of the condition number can be exponential in L and this is indeed seen in numerical experiments

With additional constraints, such as side averages, the condition number will be less but the bound is still principally the same, though possibly with (much) smaller constants. For small enough constants, the exponential growth of the condition number may no longer be apparent.

Numerical Examples

Multilevel BDDC implemented for the 2D Laplace eq. on a square domain:

2D Laplace equation results for $H_i/H_{i-1} = 8$ at all levels.

L	corners only		corners & faces		n	n_Γ
	iter	cond	iter	cond		
2	10	2.99	7	1.33	1024	240
3	19	7.30	11	2.03	65,536	15,360
4	31	18.6	13	2.72	4,194,304	983,040
5	50	47.38	15	3.40	268,435,456	62,914,560

2D Laplace equation results for $H_i/H_{i-1} = 16$ at all levels.

L	corners only		corners & faces		n	n_Γ
	iter	cond	iter	cond		
2	19	6.90	10	1.93	65,536	7936
3	23	12.62	13	2.67	1,048,576	126,976
4	43	41.43	16	3.78	268,435,456	32,505,856

2D Laplace equation results for $H_i/H_{i-1} = 4$ at all levels.

L	corners only		corners & faces		n	n_Γ
	iter	cond	iter	cond		
2	9	2.20	6	1.14	256	112
3	15	4.02	8	1.51	4096	1792
4	21	7.77	10	1.88	65,536	28,672
5	30	15.2	12	2.24	1,048,576	458,752
6	42	29.7	13	2.64	16,777,216	7,340,032

2D Laplace eq. results for $H_1/H_0 = 4$, $H_2/H_1 = 4$, and varying H_3/H_2 .

H_3/H_2	corners only		corners & faces		n	n_Γ
	iter	cond	iter	cond		
4	21	7.77	10	1.88	65,536	28,672
8	23	10.74	11	2.23	262,144	114,688
16	25	14.54	13	2.63	1,048,576	458,752
32	28	19.10	14	3.08	4,194,304	1,835,008
64	31	24.39	14	3.57	16,777,216	7,340,032

In Progress

- Multilevel BDDC in 3D, condition number bounds for linear elasticity
- Adaptive BDDC in 3D, simplified implementation, validation on real problems

Future

- Adaptive multilevel method